Numerical representation and identification of graphs [a)]

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(Received 7 January 1981; accepted for publication 24 July 1981)

A method to represent each linear graph by a single number, the determinant of its modified incidence matrix, is introduced. The isomorphism of graphs can be determined by comparing the determinants of their incidence matrices. Although it is not proved that different graphs can always be distinguished by the determinants of their modified incidence matrices, the proposed method provides a good practical algorithm for the identification of graphs. Applications of the single-number representation of graphs are discussed.

PACS numbers: 02.10.Ws, 02.70. + d

I. INTRODUCTION

Graph theory has many applications in theoretical physics. Notable examples in statistical mechanics are the Mayer's cluster expansions for the virial series of a gas,[1] and the series expansions of thermodynamic functions for spins on a lattice.[2]

In developing these perturbation expansions by graphic methods it is frequently necessary to consider the problem of identifying a graph with its isomorph in a graph list. Examples are the following.

A. Generation and listing of graphs of certain types

The first stage in graphic methods of series expansions is to obtain the list of all graphs of the type wanted. We can generate graphs of a given type by various methods. As several isomorphs (for graph terminology see Ref. 2) of a given graph may be generated, it is necessary to eliminate duplicates in the graph list. Therefore, before a new graph is added to the list we must be certain that the new graph is not isomorphic with any of the graphs already in the list.

B. Calculation of the weak embeddings

The weak embeddings $(g_i;g_j)$ are defined as the numbers of subgraphs of g_j which are isomorphic with g_i. The matrix $(g_i;g_j)$, called T-matrix by Rushbrooke,[3] plays a central role in the finite cluster method of series expansions originally suggested by Domb.[4] Another important application of the matrix $(g_i;g_j)$ is the transformation of the set of high-temperature lattice constants p_{nx} into the set of low-temperature lattice constants P_{nx}.[5] In the calculation of weak embeddings we find all subgraphs of g_j and determine which of the subgraphs are isomorphic with g_i.

C. Calculation of the coincidence partitions

The coincidence partitions $((g_n;g_m))$ are the numbers of ways of obtaining g_m by bringing some vertices of g_n into coincidence. The concept of coincidable embeddings was recently introduced by the authors.[6] The matrix $((g_n;g_m))$ transforms the set of coincidable occurrence factors C_{nx} into the set of high-temperature lattice constants p_{nx}. It is found that p_{nx} can be obtained more easily, in some cases, through such a transformation. In the calculation of $((g_n;g_m))$ we find all reduced graphs of g_n (simple graphs obtained by bringing some vertices of g_n into coincidence), and identify each reduced graph with its isomorph in a list of graphs g_m.

D. Calculation of the strong embeddings

In the calculation of the strong embeddings $[g_i;g_j]$ we find the section graphs of g_j and determine how many of the section graphs are isomorphic with g_i.

For graphs with small numbers of points (or vertices) p and lines (or edges) l, their isomorphism can be determined by visual inspection. The manual method of identification becomes laborious and fallible for even moderately complex graphs. Figure 1(a) shows a pair of isomorphs with $p = 7$ and $l = 11$; Fig. 1(b) shows a triple of isomorphs with $p = 8$ and $l = 14$. These isomorphs appear quite different and even seem to have different symmetries. It is not obvious how to identify their isomorphism by the manual method. It is very useful to devise a method to represent graphs numerically, especially when there are a large number of graphs in the list, and to determine the isomorphism and other properties of graphs by using a digital computer.

The most natural way to represent a graph of p vertices is by the use of a $p \times p$ matrix, called the incidence matrix (or adjacency matrix, see p. 14 of Ref. 2). Whether two graphs are isomorphic or not is determined by whether their incidence matrices can be transformed into one another by relabeling of the vertices. For a graph of p vertices there are $p!$ possible labelings. To compare this graph with a list of M

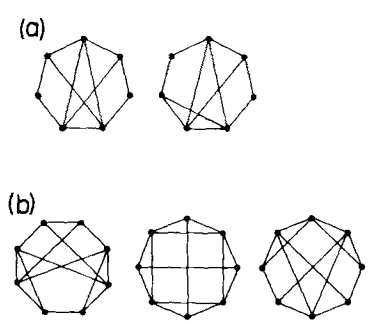

FIG. 1. (a) A pair of isomorphs of 7 points and 11 lines, and (b) a triple of isomorphs of 8 points and 14 lines. These isomorphs appear quite differently.

[a)]Work supported by the National Science Council of the Republic of China.

 0022-2488/81/122727-05$01.00

graphs the maximum number of comparisons is $Mp!$.

Nagle[7] has suggested a useful procedure for identifying graphs. Among the $p!$ matrices there exists a particular one (or several ones if the symmetry number of the graph is greater than one), called the canonical matrix, which has the largest p^2-tuple. If one first permutes the vertices to find the canonical matrix and then compares it with the list of M canonical matrices, the maximum number of comparisons is reduced to $M + p!$. A somewhat similar method of defining a canonical matrix, according to the basic key of a graph is used by Rogiers *et al.*[8] to label shadow graphs. In these matrix representations of graphs each comparison involves matrices of p^2 elements.

If we can represent each graph in the list by a single number, instead of a $p \times p$ matrix, the memory space for storing graphs, and the computing time for identifying graphs will be greatly reduced.

In Sec. II we illustrate (but do not prove) that with proper modification of the diagonal elements of the incidence matrices the determinants of the incidence matrices can be used to identify graphs. The method to represent each graph by a single number is given in Sec. III. Some applications of the single-number representation method are presented in Sec. IV. Discussions are given in Sec. V. In this article only simple graphs are considered. Extension of the single-number representation method to multigraphs (or nonsimple graphs) is straightforward.

II. DETERMINANTS OF THE MODIFIED INCIDENCE MATRICES

The incidence matrix **A** of a linear graph has elements

$a_{ij} = 1$ if vertices i and j of the graphs are connected,

$a_{ij} = 0$ otherwise. (1)

As the determinant of a matrix is the unique characteristic number of the matrix which is invariant under transformation, it is necessary that two isomorphic graphs have the same determinant. Offhand, we may expect to represent a graph by the determinant of its incidence matrix. Unfortunately, most simple graphs have $\det\mathbf{A} = 0$, because all diagonal elements and many off-diagonal elements of the matrices are zero.

The simplest modification of the incidence matrix is to add a variable x to all the diagonal elements. The modified incidence matrix $\mathbf{A}_1$ has

$$a_{ij}^{(1)} = a_{ij} + x\delta_{ij}, \tag{2}$$

where δ_{ij} is the Kronecker delta. We define functions of x for graphs g as

$$D_1(g;x) = \det\mathbf{A}_1. \tag{3}$$

The variable x or g may be omitted for convenience. D_1 are polynomials of degree p in x for graphs with p vertices.

For graphs with $p \leqslant 4$ different graphs have different D_1 functions. For $p > 5$, however, different graphs may have the same D_1 function. It is impossible to identify graphs conclusively by D_1. The function $D_1(-x)$ is nothing but the characteristic polynomial of the incidence matrix **A**. The knowledge of the function $D_1(x)$ is equivalent to the knowledge of the eigenvalues of the incidence matrix. Different graphs whose incidence matrices have the same eigenvalues, i.e., the same $D_1(x)$, are known as isospectral graphs, because these graphs have the same spectral moments.[9,10]

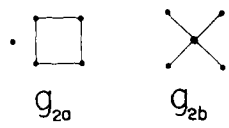

FIG. 2. Smallest pair of graphs having the same $D_1(x)$.

Figure 2 shows the smallest pairs of graphs which have the same $D_1(x)$ function. Their $D_1(x)$ functions are

$$D_1(g_{2a};x) = D_1(g_{2b};x) = x^5 - 4x^3. \tag{4}$$

The smallest pair of connected isospectral graphs[10] is shown in Fig. 3. For these graphs

$$D_1(g_{3a};x) = D_1(g_{3b};x) = x^6 - 7x^4 + 4x^3 + 7x^2 - 4x - 1. \tag{5}$$

In order to distinguish isospectral graphs we further modify the matrix and define the modified incidence matrix $\mathbf{A}_2$ by

$$a_{ij}^{(2)} = a_{ij} + (x + m_i y)\delta_{ij}, \tag{6}$$

where m_i is the vertex multiplicity (or degree) of the ith vertex of the graph, i.e., the number of lines connected to the ith vertex. Functions of x and y are defined as

$$D_2(g;x,y) = \det\mathbf{A}_2. \tag{7}$$

It is clear that D_2 are more informative than D_1. Graphs shown in Figs. 2 and 3, which have the same $D_1(x)$ can be distinguished by $D_2(x,y)$. For example,

$$D_2(g_{2a};x,y) = x(x + 2y)^2(x^2 + 4xy + 4y^2 - 4),$$

and (8)

$$D_2(g_{2b};x,y) = (x + y)^3(x^2 + 5xy + 4y^2 - 4).$$

We have surveyed more than 20 000 graphs including all graphs (connected or disconnected) with $p \leqslant 8$, and all connected graphs with $l \leqslant 11$. We find that except for two pairs of graphs shown in Figs. 4 and 5, all the graphs we considered have different $D_2(x,y)$.

For graphs shown in Figs. 4 and 5, we can further distinguish them by their functions $D_3(x,y,z) = \det\mathbf{A}_3$, where the elements of $\mathbf{A}_3$ are

$$a_{ij}^{(3)} = a_{ij} + (x + m_i y + m_i^2 z)\delta_{ij}. \tag{9}$$

We postulate that for any list of graphs there exists a number n such that all graphs in the list have different $D_n(x_1,x_2,\ldots,x_n)$ functions, although some sets of graphs may have the same $D_{n-1}(x_1,x_2,\ldots,x_{n-1})$ functions. Here D_n is the determinant

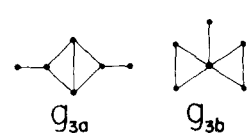

FIG. 3. Smallest pair of connected graphs having the same $D_1(x)$.

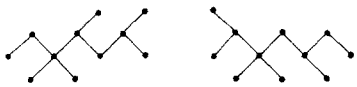

FIG. 4. Smallest pair of graphs ($l = 10$) having the same $D_2(x,y)$.

of the modified incidence matrix $\mathbf{A}_n$ having elements

$$a_{ij}^{(n)} = a_{ij} + (x_1 + m_i x_2 + m_i^2 x_3 + \cdots + m_i^{n-1} x_n)\delta_{ij}. \quad (10)$$

III. SINGLE-NUMBER REPRESENTATION OF GRAPHS

In actual practice we do not represent and identify graphs by their D_n functions explicitly. The determination of the D_n functions is complicated. Moreover, we need many coefficients to describe a D_n function. The number of coefficients required to describe the D_n function for a graph of p vertices is $(p+n)!/(p!n!)$. Although some of the coefficients are equal to zero for all simple graphs, the number of nontrivial coefficients in D_n increases rapidly with p and n.

Instead of representing a graph by a function D_n explicitly, we represent the graph by the value of D_n evaluated at a point $(x_{10},x_{20},\ldots,x_{n0})$. We first choose the point $(x_{10},x_{20},\ldots,x_{n0})$ arbitrarily, then evaluate the diagonal elements of the modified incidence matrices at this point, and finally calculate the values $D_n(g;x_{10},x_{20},\cdots)$ (to be denoted as $D_n(g)$ for convenience) directly from the matrices by standard methods such as Gauss elimination method or its variants.[11] We do not need to determine the functions D_n explicitly. All $D_n(g)$ are evaluated at the same point $(x_{10},x_{20},\ldots,x_{n0})$.

If there are N significant decimal digits in the computed results $D_n(g)$, it is certain that two graphs g_1 and g_2 are not isomorphic when $|D_n(g_1) - D_n(g_2)|/|D_n(g_1) + D_n(g_2)|$ is greater than 10^{-N}. On the other hand, if $|D_n(g_1) - D_n(g_2)|/|D_n(g_1) + D_n(g_2)|$ is less than 10^{-N}, either (i) g_1 and g_2 are isomorphic, (ii) g_1 and g_2 are not isomorphic but they have the same D_n function, or (iii) g_1 and g_2 have different D_n functions but the values $D_n(g_1)$ and $D_n(g_2)$ are degenerate "accidentally." By accidental degeneracy we mean that at the point $(x_{10},x_{20},\cdots)$ the difference between the functions $D_n(g_1)$ and $D_n(g_2)$ are too small to be distinguished by the digital computer used.

If we know by any means that accidental degeneracy does not occur, and all different graphs considered have different D_n functions, we can use a single number $D_n(g;x_{10},x_{20},\cdots)$ to represent and to identify each graph conclusively.

The probabililty P that accidental degeneracy occurs increases when the number of graphs in the list increases, or

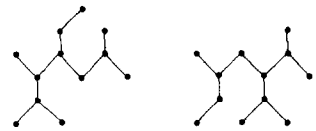

FIG. 5. Second pair of graphs ($l = 11$) having the same $D_2(x,y)$. The next pair has $l = 12$.

when the precision of the computed results decreases. If we assume that $D_n(g)$ is a random variable with uniform distribution [the actual distribution of $D_n(g)$ is probably a normal distribution with mean = 0; the probability P, however, depends very weakly on the type of distribution] it is straightforward to show that

$$P < P_u = 1 - \prod_{n=0}^{M-1} (1 - 2n/10^N), \quad (11)$$

where M is the number of graphs in the list and N is the number of significant digits in the calculation of $D_n(g)$.

Table I shows the upper bound P_u for some values of N and M. We see from Table I that even for a list of as many as 10 000 graphs the probability that accidental degeneracy occurs is about 1% if the precision in the computed results is 10 decimal digits. Such a precision can be achieved by most modern computers even without using the double precision mode. We note that when $10^N \gg M^2$, $P_u \approx M^2/10^N$.

To apply the present single-value representation method to the generation and listing of graphs we must have a simple method to check whether different graphs considered have different D_n functions, and whether accidental degeneracy does not occur at the chosen point $(x_{10},x_{20},\ldots,x_{n0})$. Fortunately, a simple method of checking does exist. Without listing all the graphs explicitly, the numbers of graphs of certain types can be determined by Polya's theorem.[1,2] For example, the total number of linear graphs among p unlabeled points with l lines, denoted by $\pi(p,l)$, the number of connected graphs, denoted by $\gamma(p,l)$, and the number of stars, $\sigma(p,l)$, etc., can be determined by Polya's theorem. If the total number of graphs of a given type obtained by the single-number representation approach is the same as that predicted by Polya's theorem, we can be certain that all graphs of the type considered have different D_n functions and accidental degeneracy does not occur.

IV. SOME APPLICATIONS

We have applied the single-number representation of graphs to the following problems:

TABLE I. Upper bounds of an approximate probability P_u see Eq. (11), that accidental degeneracy of $D_n(g)$ occurs. There are M graphs in the list and the precision of $D_n(g)$ is N digits.

N	$M = 100$	500	1000	5000	10 000	50 000
6	0.985E-2	0.221	0.632	~1		
7	0.989E-3	0.246E-1	0.951E-1	0.918	~1	
8	0.990E-4	0.249E-2	0.994E-2	0.221	0.632	~1
9	0.990E-5	0.249E-3	0.998E-3	0.247E-1	0.952E-1	0.918
10	0.990E-6	0.249E-4	0.999E-4	0.249E-2	0.995E-2	0.221
11	0.990E-7	0.249E-5	0.999E-5	0.250E-3	0.999E-3	0.247E-1

A. Generation and listing of graphs (connected and disconnected) with $p \leqslant 8$

All p-point graphs can be generated by adding 0 to $p-1$ lines from the pth vertex to $(p-1)$-point graphs. We input $(p-1)$-point graphs, one at a time, to the memory of the computer and generate several p-point graphs from each input graph. Since graphs with different l or p are not isomorphic, isomorphism needs to be checked only for graphs with the same values of l and p. We represent and identify graphs by $D_2(x_0,y_0)$ at $x_0 = 1.234\,567$ and $y_0 = 0.111\,111\,1$. When several graphs generated have the same p, l, and $D_2(x_0,y_0)$, only the first one is listed, the others are eliminated. When a graph is listed only its D_2 value is stored in the memory; the incidence matrix of the graph is then transferred from the memory to an output device. The total numbers of different graphs we obtained are $\pi(p) = 2, 4, 11, 34, 156, 1044$, and 12 346, respectively for $p = 2$–8. These numbers are the same as those predicted by Polya's theorem. The computing time used to obtain these graphs is about 1200 seconds for a CDC Cyber 172 computer.

B. Generation and listing of connected graphs with $l \leqslant 11$

All the p-point, l-line connected graphs can be obtained by adding n lines $(0 < n < p)$ from the pth vertex to the $(p-1)$-point, $(l-n)$-line graphs. The first time we used $D_2(x_0,y_0)$ to identify graphs. When we compared the numbers of graphs of various sizes with those predicted by Polya's theorem, we found that two graphs were absent in our graph list.

Polya's theorem predicts that the number of connected graphs with $p = 11$ and $l = 10$ is $\gamma(11,10) = 235$, but the number of graphs of this type we obtained is 234. We can expect that among the 235 graphs either two of them have the same D_2 function, or their D_2 functions are degenerate accidentally at (x_0,y_0). Similarly the number of connected graphs we obtained with $p = 12$ and $l = 11$ is 550, while the correct number is $\gamma(12,11) = 551$.

A CDC Cyber 172 computer was used in our calculation. The precision of this computer is 14 decimal digits for the single-precision mode, and the computed results $D_n(g)$ are expected to have 12 significant decimal digits. For a list of $M = 551$ graphs the probability that accidental degeneracy occurs is less than 10^{-6} (see Table I). We can be almost sure from this probability that accidental degeneracy does not occur.

We then used $D_3(x_0,y_0,z_0)$ at $x_0 = 1.234\,567$, $y_0 = 0.111\,111\,1$, and $z_0 = 0.054\,321$ to identify graphs; and we obtained the correct number of graphs. With the complete list of graphs it is easy to locate the pairs of graphs which cannot be distinguished by $D_2(x_0,y_0)$. They are shown in Figs. 4 and 5. We calculated the D_2 functions of these graphs explicitly. As expected, the graphs shown in Fig. 4 have the same D_2 function, and so do the graphs in Fig. 5. The numbers of l-line connected graphs for l equal 1 through 11 are 1, 1, 3, 5, 12, 30, 79, 227, 710, 2322, and 8071, respectively. To obtain these graphs, when graphs are identified by D_3, the computing time is about 1850 seconds.

C. Calculation of coincidence partitions $((g_n;g_m))$

In a previous paper we derived the high-temperature lattice constants for a generalized equivalent neighbor model.[6] In this paper the matrix element $((g_n;g_m))$ for stars with $l \leqslant 8$ was derived by a manual method. We have recently calculated the low-temperature lattice constants for this model.[12] The procedures for deriving the elements $((g_n;g_m))$ have been computerized, and the matrix has been derived to the seventh order, i.e., for all connected graphs with $p \leqslant 7$. There are two procedures in the calculation: to obtain all reduced graphs of g_n, and to identify each reduced graph with its isomorph in the list g_m. We identified graphs by $D_2(x_0 = 1.234\,567, y_0 = 0.111\,111\,1)$. The computing time for deriving the matrix to the seventh order is about 5200 seconds for a CDC Cyber 172 computer. It would take more than 5000 hours to obtain these matrix elements manually.

V. DISCUSSION

We have introduced a method to represent a p-point graph g by a single number $D_n(g)$, instead of a $p \times p$ incidence matrix **A**. For each graph $D_n(g)$ is the determinant of its modified incidence matrix $\mathbf{A}_n$ whose diagonal elements depend on the numbers of lines connected to the vertices.

In previous matrix-representation methods each graph is represented by a matrix. A memory space of Mp^2 words is required to store M graphs. In the present method each graph is represented by a single number. A memory space of M words is enough for the M graphs. The memory space is reduced p^2-fold. Although it is possible to store several numbers simultaneously in each word when very low precision is sufficient (such as the elements of the canonical matrices), the memory space required for storing a matrix is much larger than that for storing a number. Furthermore, the saving of memory space by storing several numbers in one word must be compensated for by an increase of computation time.

For a graph of p vertices there are $p!$ matrices corresponding to the $p!$ different labelings of the vertices. One can permute the vertices to find the canonical matrix out of the $p!$ matrices. Nagle[7] has illustrated a method to write down the canonical matrix of a graph in an easier way than actually constructing all the permissible matrices. The vertices are first relabeled so that $m_1 \geqslant m_2 \geqslant m_3 \cdots \geqslant m_p$. One then permutes only the vertices which have the same degree, and determines the canonical matrix. In the present method we simply modify the diagonal elements of the incidence matrix, and then evaluate the determinant $D_n(g)$. The computing time in the calculation of the determinant is proportional to p^3 if the Gauss elimination method is used.[11] When p is small (say $p \leqslant 6$) or when most of the vertices in a graph have different degrees, the computing time for finding the determinant may be longer than that for finding the canonical matrix. Otherwise the time required to evaluate D_n is expected to be shorter.

As far as the graph identification is concerned, we compare a number to a list of M numbers, while in the previous methods one compares a matrix to a list of M matrices. The computing time is reduced considerably in the present method.

For moderately complex graphs, $D_2(x_0,y_0)$ can be used to identify graphs. For more complex graphs, D_3 or higher-order ones should be used. It is important to note that when we use either D_2 or D_3 to identify graphs, the difference in computing time is about 1%. Even when we use D_4 or D_5, the increase of computing time is only a few percent.

The values x_0, y_0, etc., may be chosen arbitrarily, but integers are not recommended. The probability that the values of two different D_n functions are too close to be distinguished by a computer is very small. Even so, when we apply the present method to the generation and listing of graphs we must check whether the total number of graphs we obtained is correct. Should the total number be incorrect, we have to try other values $(x_0,y_0,\cdots)$, or try a higher-order D_n.

We can also define different kinds of modified incidence matrices whose diagonal elements are more complicated functions of m_i (instead of polynomials in m_i). However, when using more complicated functions it takes a longer time to evaluate the diagonal elements.

In Sec. IV we have applied the present single-number representation method to the generation and listing of graphs, and to the calculation of graph embeddings. There are other applications. We can identify isospectral graphs by comparing their $D_1(x_0)$ numerically. We can determine numerically whether a graph is connected or disconnected. Consider graphs g_1, g_2, and g_3 which have numbers of vertices p_1, p_2, and p_3, respectively. If $p_1 = p_2 + p_3$ and $D_n(g_1) = D_n(g_2)D_n(g_3)$, then g_1 is a disconnected graph composed of g_2 and g_3, provided all graphs with the same number of vertices can be distinguished by D_n.

In conclusion, we have introduced a method to represent each graph by a single number, instead of a canonical matrix. Both the memory space for storing graphs in a computer and the computing time for identifying graphs are greatly reduced, especially for complex graphs. Finally, we hope that someone will prove the postulate that for any list of graphs there exists an integer n such that all graphs in the list have different D_n functions.

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Sp(6) states in an SU(3)×U(1) basis [a)]

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(Received 19 May 1981; accepted for publication 1 August 1981)

We find all missing label operators and also a complete set of analytic nonorthonormal basis states for the group–subgroup Sp(6)⊃SU(3)×U(1), both for the compact version of Sp(6) and for the noncompact Sp(6,R) relevant to the symplectic nuclear collective model.

PACS numbers: 02.20. + b, 21.60.Ev, 21.60.Fw

1. INTRODUCTION

The symplectic nuclear collective model[1] combines the features of the Bohr–Mottelson and of the Elliott models. The nuclear states are classified as bases of irreducible representations[2] of the noncompact group Sp(6,R), reduced according to its SU(3)×U(1) subgroup. The subgroup does not provide enough labels to specify the states uniquely—the same SU(3)×U(1) representation may occur many times in one Sp(6,R) representation. The same is true for the compact group Sp(6) reduced according to its subgroup SU(3)×U(1). Racah's counting of labels[3] gives the number of missing labels as three in both cases.

One method of resolving the multiplicity problem is the use of basis states which are common eigenstates of some complete set of commuting Hermitian operators.[4] Besides the Casimir operators of group and subgroup, and appropriate internal subgroup labels, three additional labeling operators must be found. These missing label operators should be subgroup scalars in the enveloping algebra of the group, i.e., polynomials in the group generators. In Sec. 2 we derive a generating function for SU(3)×U(1) scalars in the enveloping algebra of Sp(6). It provides an integrity basis—a small number of elementary subgroup scalars in terms of which all can be expressed as products. The generating function is the same for compact and noncompact Sp(6).

Another approach to the labeling problem is to define a complete linearly independent set of analytic, but nonorthonormal, basis states. In Sec. 3 we find generating functions for Sp(6)⊃SU(3)×U(1) branching rules for the compact and the noncompact cases. They provide basis states for all relevant representations of Sp(6) in terms of a small number of elementary multiplets.

Section 4 contains some concluding remarks.

2. MISSING LABEL OPERATORS

The objective of this section is to enumerate all SU(3)×U(1) scalars which are polynomials in the Sp(6) generators. Since they commute with the Casimir operators, and internal subgroup labels, they may serve as missing label operators.

The generators of Sp(6), compact or noncompact, break up under SU(3)×U(1) into an octet U and a singlet D, both with U(1) weight 0, and a sextet V and an antisextet W with U(1) weights ± 1, respectively. The SU(3) generators are the components of the octet U; the singlet D is the U(1) generator.

Our strategy is to find two generating functions for SU(3) polynomial tensors, one in the components of U, the other in the components of V and W, and then to combine them to obtain a generating function for SU(3)×U(1) scalars which are polynomials in all the generators. For a discussion of the use of generating functions in connection with representations of Lie groups, see Refs. 5,6.

The generating function for polynomial SU(3) tensors in the components of the octet U is known to be[5]

$$G_1(U,A,B) = \frac{1 + U^2AB + U^4A^2B^2}{(1-U^2)(1-U^3)(1-UAB)(1-U^3A^3)(1-U^3B^3)}. \tag{2.1}$$

A term $U^uA^aB^bC_{uab}$ in the expansion of (2.1) implies that there are C_{uab} tensors of type (a,b) among the terms of degree u in U. These tensors all have U(1) weight 0.

Similarly the generating functions for SU(3) polynomial tensors in V and W are[7]

$$G_2(V,A,B) = [(1-VA^2)(1-V^2B^2)(1-V^3)]^{-1} \tag{2.2}$$

and

$$G_3(W,A,B) = [(1-WB^2)(1-W^2A^2)(1-W^3)]^{-1}, \tag{2.3}$$

respectively. A tensor of degree v in V carries the U(1) weight v; one of degree w in W has U(1) weight $-w$.

A U(1) scalar must have V and W occurring to the same degree. To extract the U(1) scalar part of the product of G_2 and G_3 we therefore write

$$G_2(V,A_1,B_1)G_3(YV^{-1},A_2,B_2)$$

and retain only terms of degree 0 in V. Denote the result by $H(Y,A_1,B_1,A_2,B_2)$. Then Y carries as its exponent the common degree in V and W. The labels of SU(3) representations arising from V are carried by A_1,B_1, those from W by A_2,B_2. The direct products of the tensors from V with those from W are conveniently taken with the help of the SU(3) Clebsch–Gordan generating function[6]

a)Work supported in part by the Natural Science and Engineering Research Council of Canada and by the Ministère de l'Education du Québec.

 0022-2488/81/122732-04$01.00

$$C(A_1,B_1,A_2,B_2,A,B)$$
$$= [(1-A_1A)(1-B_1B)(1-A_2A)$$
$$\times(1-B_2B)(1-A_1B_2)(1-B_1A_2)]^{-1} \quad (2.4)$$
$$\times\{(1-A_1A_2B)^{-1}+B_1B_2A(1-B_1B_2A)^{-1}\}.$$

Writing $H(Y,A_1,B_1,A_2,B_2)C(A_1^{-1},B_1^{-1},A_2^{-1},B_2^{-1},A,B)$ and retaining only terms of degree 0 in A_1,B_1,A_2,B_2 we obtain $J(Y,A,B)$ which enumerates SU(3) tensors (labels carried by A and B) of equal degree (carried by Y) in V and W.

Finally, we write the product $G_1(U,A,B)J(Y,B^{-1},A^{-1})$ and extract the part of degree 0 in A and B. Multiplying by $(1-D)^{-1}$ to take account of the U(1) generator we obtain the generating function

$$K(U,Y,D) = [(1-Y)(1-Y^2)$$
$$\times(1-Y^3)(1-U^2)(1-U^3)(1-D)$$
$$\times(1-UY)(1-U^2Y)^2(1-UY^2)(1-U^3Y)]^{-1} \quad (2.5)$$
$$\times\{(1+2U^2Y^2+2U^2Y^3+U^2Y^4+2U^3Y^2+3U^2Y^3$$
$$+U^3Y^4+2U^4Y^2+2U^4Y^3$$
$$+3U^4Y^4+U^4Y^6+U^5Y^5+U^5Y^6)$$
$$\times(1-U^2Y^2)^{-1}+(U^4Y+U^4Y^2+U^4Y^3+U^4Y^5$$
$$+U^5Y^2+U^5Y^3+U^5Y^4+U^5Y^5+U^6Y^2+3U^6Y^3$$
$$+3U^6Y^4+2U^6Y^5+U^7Y^3+2U^7Y^4+U^7Y^5+U^8Y^3$$
$$+2U^8Y^4+3U^8Y^5+U^{10}Y^7)(1-U^4Y)^{-1}\}.$$

for SU(3)×U(1) scalars in the Sp(6) enveloping algebra.

The first six denominator factors in (2.5) correspond to the Casimir operators of Sp(6), SU(3), and U(1). Omitting these factors, we have a generating function for missing label operators. Since there are three missing labels, we expect six functionally independent label operators[8]; this accords with the fact that, apart from the six Casimir operators, each term of (2.5) contains six denominator factors.

The generating function (2.5) may be interpreted in terms of an integrity basis—a finite number, 31 in this case, of elementary labeling operators in terms of which all may be written as products. Some combinations of elementary operators are incompatible—their products are redundant because they can be expressed as linear combinations of other products. Equation (2.5) specifies the elementary labeling operators by giving their degrees in U,V, and W [Y in (2.5) could be replaced by VW]; from that information it is easy to construct them. For example the operator designated by UY is

$$\sum_{ijk} V_i U_j W_k \begin{pmatrix} 20 & 11 & 02 \\ i & j & k \end{pmatrix}. \quad (2.6)$$

The coefficient in (2.6) is an SU(3) Wigner coefficient. The two operators corresponding to U^2Y are

$$\sum_{ijklm} V_i U_j U_k W_l \begin{pmatrix} 20 & 02 & 22 \\ i & l & m \end{pmatrix}\begin{pmatrix} 11 & 11 & 22 \\ j & k & m \end{pmatrix} \quad (2.7)$$

and

$$\sum_{ijklm} V_i U_j U_k W_l \begin{pmatrix} 20 & 02 & 11 \\ i & l & m \end{pmatrix}\begin{pmatrix} 11 & 11 & 11 \\ j & k & m \end{pmatrix}. \quad (2.8)$$

The triangular bracket symbols in (2.7) and (2.8) are SU(3) Clebsch–Gordan coefficients; the SU(3) Wigner coefficient in (2.8) describes the symmetric coupling of three octets to give a scalar.

The phases of the generators V and W may be chosen so that their commutation rules are the same for compact and noncompact Sp(6); then the components of W, when written in terms of the Hermitian conjugates of the components of V, have opposite signs in the two cases. Corresponding compact and noncompact labeling operators may differ by a factor i in order that both be Hermitian.

There remains the problem of choosing three missing label operators which mutually commute. We hope to return to this question soon. In the meantime, a single labeling operator, or if necessary, an irrational linear combination of operators from the integrity basis implied by (2.5) will probably suffice to resolve any degeneracy of practical interest.

Couture and Sharp[9] have given a generating function [their Eq. (5.3)] for Sp(6) tensors contained in the Sp(6) enveloping algebra. According to (3.7) each Sp(6) tensor whose representation labels are all even contains just one SU(3)×U(1) scalar. Hence the even-even-even part of (5.3) of Ref. 9 is a generating function for SU(3)×U(1) scalars in the Sp(6) enveloping algebra. Our (2.5) is preferable since it gives the degrees of the scalars in U, V, W, and D separately.

3. ANALYTIC Sp(6)⊃SU(3)×U(1) BASIS STATES

In this section we give generating functions for branching rules for noncompact and compact Sp(6) reduced according to SU(3)×U(1). In each case the generating function is interpreted in terms of analytic Sp(6)⊃SU(3)×U(1) basis states.

The basis states of the discrete series of irreducible representations of noncompact Sp(6,R) required for the symplectic nuclear collective model are generated[1] by applying polynomials in the components of an SU(3) sextet Z of unit U(1) weight to the states of an SU(3)×U(1) irreducible representation $(p,q;d)$. The components of the sextet Z are two-quantum creation operators: the U(1) weight z is the initial weight d plus one-half the number of quanta present.

According to (2.2) the generating function for SU(3)×U(1) representations generated by the sextet Z is

$$G_2(Z,A,B) = [(1-ZA^2)(1-Z^2B^2)(1-Z^3)]^{-1}. \quad (3.1)$$

A and B in (3.1) carry the SU(3) representation labels and Z carries the U(1) weight. Let us denote the six states of the sextet Z by

$$\alpha = |2,2\rangle, \quad \beta = |2,1\rangle, \quad \gamma = |2,0\rangle,$$
$$\delta = |2,-1\rangle, \quad \epsilon = |2,-2\rangle, \quad \theta = |0,0\rangle. \quad (3.2)$$

The notation is $|L,M\rangle$ where L and M label the states of the O(3) subgroup of SU(3). The generating function (3.1) implies an integrity basis of three elements. The first is the basic sextet with highest component α: the second is an antisextet with highest component

$$G = 2(\sqrt{2})\alpha\gamma - (\sqrt{3})\beta^2 - 2\alpha\theta. \quad (3.3)$$

The third is an SU(3) scalar

$$S = -3(\sqrt{3})\alpha\delta^2 - 3(\sqrt{3})\beta^2\epsilon - (\sqrt{2})\gamma^3 + 3(\sqrt{2})\beta\gamma\delta + 6(\sqrt{2})\alpha\epsilon\gamma - 6\alpha\epsilon\theta + 6\beta\delta\theta - 3\gamma^2\theta + 2\theta^3. \quad (3.4)$$

The highest component of the SU(3) tensor (x,y) generated by Z is given explicitly by

$$|2a,2b,a+2b+3c;\,2a+2b,\,2a+2b\rangle = \alpha^a G^b S^c, \quad (3.5)$$

where we have used the notation $|x,y,z;L,M\rangle$. The tensors defined by (3.5) can now be coupled to the basic SU(3)×U(1) multiplet $(p,q;d)$, which defines the Sp(6,R) representation under consideration, with the help of SU(3) Clebsch–Gordan coefficients to give analytic Sp(6,R)⊃SU(3)×U(1) basis states. Such states are suitable for the evaluation of Sp(6,R) generator matrix elements and Clebsch–Gordan coefficients in an SU(3)×U(1) basis.

A generating function for Sp(6,R)⊃SU(3)×U(1) branching rules is obtained by multiplying $G_2(Z,A_1,B_1)$, given by (3.1), by $[(1-PA_2)(1-QB_2)(1-ZD)]^{-1}$ and by the SU(3) Clebsch–Gordan generating function $C(A_1^{-1},B_1^{-1},A_2^{-1},B_2^{-1},A,B)$ defined in (2.4), and retaining the part of degree 0 in A_1,A_2,B_1,B_2. The result is

$$\begin{aligned}
&F_1(P,Q,D;A,B,Z)\\
&\quad=[(1-ZA^2)(1-Z^2B^2)(1-PA)(1-QB)\\
&\quad\times(1-ZQ^2)(1-Z^2P^2)(1-ZD)(1-Z^3)]^{-1}\\
&\quad\times[(1+QAZ+PABZ+PQBZ)(1+PBZ^2)/\\
&\quad(1-P^2B^2Z)\\
&\quad+(QABZ^2+PQAZ^2+Q^2A^2Z^2+PQ^2A^2BZ^4)\\
&\quad\times(1+QAZ)/(1-Q^2A^2Z^2)]. \qquad (3.6)
\end{aligned}$$

A term $P^pQ^qD^dA^aB^bZ^zC_{pqdabz}$ in the expansion of (3.6) implies that the SU(3)×U(1) representation $(a,b;z)$ appears C_{pqdabz} times in the Sp(6,R) representation $(p,q;d)$. The fact that there are nine denominator factors in each term of (3.6), three more than the number of group and subgroup labels, implies three missing labels, in agreement with Racah's counting.[3]

We now turn to the generating function for branching rules for compact Sp(6) reduced according to SU(3)×U(1). In principle the generating function could be computed analytically starting with the Sp(6) character generator.[10] To avoid tedious algebra we use instead the method of elementary multiplets.

By examining the SU(3)×U(1) content of a number of low-lying Sp(6) irreducible representations,[11] we may infer the integrity basis for the problem. It is a finite set of SU(3)×U(1) multiplets contained in low Sp(6) representations, in terms of which all may be expressed as stretched products. Written as a generating function the result takes the form

$$\begin{aligned}
&F_2(K,L,M;A,B,Z)\\
&=\left[\frac{1+KMAB}{(1-K^2)(1-MA^2Z^{-1})(1-MB^2Z)}+\frac{L^2}{(1-K^2)(1-L^2)(1-KLAZ)}+\frac{KL^3BZ^{-1}}{(1-K^2)(1-L^2)(1-KLBZ^{-1})}\right.\\
&+\frac{L^4A^2Z^2}{(1-L^2A^2Z^2)(1-L^2)(1-KLAZ)}+\frac{L^4B^2Z^{-2}}{(1-L^2)(1-L^2B^2Z^{-2})(1-KLBZ^{-1})}\\
&+\frac{LAB}{(1-LAB)(1-L^2A^2Z^2)(1-L^2)}+\frac{L^3AB^3Z^{-2}}{(1-LAB)(1-L^2B^2Z^{-2})(1-L^2)}\\
&+\frac{LM^2A^3B^3}{(1-LAB)(1-MA^2Z^{-1})(1-MB^2Z)}+\frac{LMA^3BZ^{-1}}{(1-LAB)(1-L^2A^2Z^2)(1-MAZ^{-1})}\\
&+\frac{LMAB^3Z}{(1-LAB)(1-L^2B^2Z^{-2})(1-MB^2Z)}+\frac{KLAZ}{(1-K^2)(1-MA^2Z^{-1})(1-KLAZ)}\\
&+\frac{KLBZ^{-1}}{(1-K^2)(1-MB^2Z)(1-KLBZ^{-1})}+\frac{L^2A^2Z^2}{(1-L^2A^2Z^2)(1-MA^2Z^{-1})(1-KLAZ)}\\
&\left.+\frac{L^2B^2Z^{-2}}{(1-L^2B^2Z^{-2})(1-MB^2Z)(1-KLBZ^{-1})}\right]\\
&[(1-KAZ)(1-KBZ^{-1})(1-LBZ^2)(1-LAZ^{-2})(1-MZ^3)(1-MZ^{-3})]^{-1}. \qquad (3.7)
\end{aligned}$$

The dummy variables K,L,M carry the Sp(6) representation labels as exponents, while A,B,Z carry the SU(3) and U(1) labels. For example the coefficient of KL in the expansion of (3.7), namely $ABZ^3+A^2BZ+B^2Z+AZ+BZ^{-1}+A^2Z^{-1}+AB^2Z^{-1}+ABZ^{-3}$ tells us that the SU(3)×U(1) content of (110) is (11,3) + (21,1) + (02,1) + (10,1) + (01, − 1) + (20, − 1) + (12, − 1) + (11, − 3).

The validity of (3.7) was checked by converting it, by appropriate substitutions, into a generating function for Sp(6) weights. It was then compared with the generating function for weights obtained from the known[12] Sp(6)⊃Sp(4)×SU(2) generating function. Since an analytic comparison of the two versions of the Sp(6) character (weight) generator would be very laborious, we made the necessary substitutions by means of a computer program and compared the two generating functions at random values of their arguments.

The generating function (3.7) implies a set of polynomial bases for compact Sp(6)⊃SU(3)×U(1). First one evaluates

the highest states of the elementary multiplets as polynomials in the states of the fundamental irreducible representations (100), (010), and (001). Compatible products of powers of these highest states correspond one-to-one to highest states of all $SU(3)\times U(1)$ multiplets contained in Sp(6) representations. Unwanted admixtures of states belonging to lower Sp(6) representations than the degree of the polynomials would suggest may be eliminated by the techniques of Lohe and Hurst.[13]

4. CONCLUDING REMARKS

The results of this paper suggest some areas for further work.

An obvious problem, mentioned in Sec. 2, is that of finding three commuting functions of the six functionally independent missing label operators provided by the generating function (2.5). We conjecture that a general solution of the problem might go somewhat along the following lines. Choose, on grounds of mathematical or empirical convenience, one missing label operator. Impose on an unknown function of the other five that it commute with the chosen one. That condition will determine four independent functions from which the next label operator must be chosen. At each stage of selection there are twice as many operators available as are still needed. Such a general procedure may be overly ambitious. For the moment we would be happy to have one set of three commuting label operators.

The analytic basis states for noncompact $Sp(6,R)\supset SU(3)\times U(1)$ could be used to derive quite general generator matrix elements and $Sp(6,R)\supset SU(3)\times U(1)$ reduced Wigner coefficients. These would have application to the symplectic nuclear collective model.

ACKNOWLEDGMENT

We thank J. Patera and D. J. Rowe for helpful discussions.

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Generating functions for G_2 characters and subgroup branching rules [a)]

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(Received 22 April 1981; accepted for publication 31 July 1981)

The G_2 character generator is given; with its help generating functions are derived for branching rules for G_2 irreducible representations reduced according to its maximal semisimple subgroups.

PACS numbers: 02.20.Hj

I. INTRODUCTION

The character generator of a simple group, apart from providing the characters, or weights, or all irreducible representations, turns out to be a convenient starting point for the calculation of other generating functions, for example, for branching rules to a semisimple or finite subgroup or for direct products of representations of the group.

A few character generators, or the equivalent integrity bases, have been known for some time.[1,2] Recently R. P. Stanley[3] has derived the SU(n) character generator; and R. C. King[4] has given the character generator for Sp($2n$).

In Sec. II we derive the character generator for the exceptional group G_2, and with its help, in Secs. III and IV, we obtain generating functions for the branching rules of G_2 to its maximal semisimple subgroups SU(2)×SU(2) and O(3); the generating function for $G_2 \supset$ SU(3) branching rules appears in Eq. (2.3). Section V contains some additional comments.

II. THE G_2 CHARACTER GENERATOR

The G_2 character generator is defined by its power series expansion

$$H(A,B;\eta,\xi) = \sum_{abmn} A^a B^b \eta^m \xi^n C_{ab,mn}, \tag{2.1}$$

where $C_{ab,mn}$ is the multiplicity of the weight (m,n) in the G_2 representation (ab).

To derive an explicit formula for $H(A,B;\eta,\xi)$ we "substitute" the SU(3) character generator into the generating function for $G_2 \supset$ SU(3) branching rules.

The SU(3) character generator is known to be[1,2]

$$\begin{aligned} &G(P,Q;\eta,\xi) \\ &= [(1-P\eta\xi)(1-P\eta^{-1}\xi)(1-Q\eta\xi^{-1})(1-Q\eta^{-1}\xi^{-1})]^{-1} \\ &\quad \times [(1-P\xi^{-2})^{-1} + (1-Q\xi^2)^{-1}Q\xi^2]. \end{aligned} \tag{2.2}$$

The component of weight carried as exponent by the dummy variable η in (2.2) is twice the component of isospin, while that carried by ξ is three times the hypercharge. The generating function for $G_2 \supset$ SU(3) branching rules is[5,6]

$$\begin{aligned} F(A,B;P,Q) &= [(1-AP)(1-AQ)(1-BP)(1-BQ)]^{-1} \\ &\quad \times [(1-A)^{-1} + (1-BPQ)^{-1}BPQ]. \end{aligned} \tag{2.3}$$

The coefficient of $A^a B^b P^p Q^q$ in the expansion of (2.3) is the multiplicity of the SU(3) representation (p,q) in the G_2 representation (a,b).

The G_2 character generator is found by retaining the terms of zero degree in P and Q in the product $F(A,B;P,Q)G(P^{-1},Q^{-1};\eta,\xi)$. The result of this operation is

$$\begin{aligned} H(A,B;\eta,\xi) &= H_1(A,B;\eta,\xi) + H_1(A,B;\eta^{-1},\xi) \\ &\quad + H_2(A,B;\eta,\xi) + H_2(A,B;\eta^{-1},\xi) \\ &\quad + H_2(A,B;\eta,\xi^{-1}) + H_2(A,B;\eta^{-1},\xi^{-1}), \end{aligned} \tag{2.4}$$

where

$$\begin{aligned} H_1(A,B;\eta,\xi) &= [(1-A\eta\xi)(1-A\eta\xi^{-1})(1-B\eta\xi)(1-B\eta\xi^{-1}) \\ &\quad \times (1-\eta^{-2})(1-\eta^{-1}\xi^3)(1-\eta^{-1}\xi^{-3})]^{-1} \\ &\quad \times [(1-A)^{-1}A + (1-B\eta^2)^{-1}], \\ H_2(A,B;\eta,\xi) &= [(1-A\eta\xi)(1-A\xi^2)(1-B\eta\xi)(1-B\xi^2) \\ &\quad \times (1-\eta^{-2})(1-\eta\xi^{-3})(1-\eta^{-1}\xi^{-3})]^{-1} \\ &\quad \times [(1-A)^{-1}A + (1-B\eta\xi^3)^{-1}]. \end{aligned} \tag{2.6}$$

The right-hand side of (2.4) reduces to the final form

$$\begin{aligned} H(A,B;\eta,\xi) &= [(1-A\xi^2)(1-A\xi^{-2})(1-B\eta\xi^3)(1-B\eta^{-1}\xi^{-3})]^{-1} \\ &\quad \times \{(1+A)[(1-A\eta\xi)(1-A\eta\xi^{-1})(1-A\eta^{-1}\xi)(1-A\eta^{-1}\xi^{-1})]^{-1} \\ &\quad + B\eta^2[(1-A\eta\xi)(1-A\eta\xi^{-1})(1-A\eta^{-1}\xi^{-1})(1-B\eta^2)]^{-1} \\ &\quad + B\eta^{-2}[(1-A\eta\xi)(1-A\eta^{-1}\xi)(1-A\eta^{-1}\xi^{-1})(1-B\eta^{-2})]^{-1} \\ &\quad + B\eta\xi^{-3}(1+A)[(1-A\eta\xi)(1-A\eta\xi^{-1})(1-A\eta^{-1}\xi)(1-B\eta\xi^{-3})]^{-1} \\ &\quad + B\eta^{-1}\xi^3(1+A)[(1-A\eta\xi^{-1})(1-A\eta^{-1}\xi)(1-A\eta^{-1}\xi^{-1})(1-B\eta^{-1}\xi^3)]^{-1} \\ &\quad + B^2\eta^3\xi^{-3}[(1-A\eta\xi)(1-A\eta\xi^{-1})(1-B\eta\xi^{-3})(1-B\eta^2)]^{-1} \end{aligned}$$

[a)]Work supported in part by the Natural Science and Engineering Research Council of Canada and by the Ministère de l'Education du Québec.

 0022-2488/81/122736-04$01.00

$$
\begin{aligned}
&+B^2\eta^{-3}\xi^3[(1-A\eta^{-1}\xi)(1-A\eta^{-1}\xi^{-1})(1-B\eta^{-1}\xi^3)(1-B\eta^{-2})]^{-1}\\
&+(B^2\eta\xi^3+A^2B(1+\eta\xi^{-1}))[(1-A\eta\xi^{-1})(1-A\eta^{-1}\xi^{-1})(1-B\eta^{-1}\xi^3)(1-B\eta^2)]^{-1}\\
&+(B^2\eta^{-1}\xi^{-3}+A^2B(1+\eta^{-1}\xi))[(1-A\eta\xi)(1-A\eta^{-1}\xi)(1-B\eta\xi^{-3})(1-B\eta^{-2})]^{-1}\\
&+(B^2+A^2B)[(1-A\eta\xi)(1-A\eta^{-1}\xi^{-1})(1-B\eta^2)(1-B\eta^{-2})]^{-1}\\
&+(B^2+AB^2)[(1-A\eta\xi^{-1})(1-A\eta^{-1}\xi)(1-B\eta\xi^{-3})(1-B\eta^{-1}\xi^3)]^{-1}\\
&+(B^3\eta^2+AB(\eta^2+\eta\xi))[(1-A\eta\xi^{-1})(1-B\eta\xi^{-3})(1-B\eta^{-1}\xi^3)(1-B\eta^2)]^{-1}\\
&+(B^3\eta^{-2}+AB(\eta^{-2}+\eta^{-1}\xi^{-1}))[(1-A\eta^{-1}\xi)(1-B\eta\xi^{-3})(1-B\eta^{-1}\xi^3)(1-B\eta^{-2})]^{-1}\\
&+(B^3\eta\xi^{-3}+AB(1+\eta^2+\eta\xi+\eta\xi^{-1})+AB^2\eta\xi^{-1})[(1-A\eta\xi)(1-B\eta\xi^{-3})(1-B\eta^2)(1-B\eta^{-2})]^{-1}\\
&+(B^3\eta^{-1}\xi^3+AB(1+\eta^{-2}+\eta^{-1}\xi^{-1}+\eta^{-1}\xi)+AB^2\eta^{-1}\xi)\\
&\times[(1-A\eta^{-1}\xi^{-1})(1-B\eta^{-1}\xi^3)(1-B\eta^2)(1-B\eta^{-2})]^{-1}\\
&+B(1+B)(B^2+2+\xi^2+\xi^{-2}+\eta\xi+\eta\xi^{-1}+\eta^{-1}\xi+\eta^{-1}\xi^{-1})\\
&\times[(1-B\eta\xi^{-3})(1-B\eta^{-1}\xi^3)(1-B\eta^2)(1-B\eta^{-2})]^{-1}\}. \qquad (2.7)
\end{aligned}
$$

The coefficient of $A^aB^b\eta^m\xi^n$ in the expansion of (2.7) is the multiplicity of the G_2 (or SU(3)) weight (m,n) in the G_2 representation (a,b).

III. $G_2 \supset SU(2)\times SU(2)$ BRANCHING RULES

Stone[7] has given an explicit formula for the $SU(2)\times SU(2)$ content of G_2 representations. His formula involves plus and minus signs, with consequent cancellations. An advantage of our generating function formulation is that the terms are all positive and in that sense it is more economical. Also it defines an integrity basis—a finite set of elementary $SU(2)\times SU(2)$ multiplets contained in low-lying G_2 representations. All $SU(2)\times SU(2)$ multiplets in all G_2 representations can be expressed in terms of stretched products of powers of the elementary ones; such products of powers of elementary multiplets define polynomial bases for G_2 in an $SU(2)\times SU(2)$ basis.

The $G_2 \supset SU(2)\times SU(2)$ generating function could be determined analytically[6] from the G_2 character generator (2.7). It is the part $J(A,B;S,T)$ of degree zero in η and ξ of the product $H(A,B;\eta,\xi)(1-\eta^2)(1-\xi^2)[(1-S\eta)(1-T\xi)]^{-1}$. To avoid tedious algebra we constructed it heuristically by examining[8] the $SU(2)\times SU(2)$ content of low G_2 representations. It was then converted back to a generating function for weights by substituting the $SU(2)\times SU(2)$ character function. It was then compared with (2.7) for random values of the dummy variables A, B, η, ξ. Our result is

$$
\begin{aligned}
&J(A,B;S,T)\\
&=[(1-AST)(1-AT^2)(1-BS^2)(1-B^2)]^{-1}\\
&\times\{(1+A^2ST+A^2BST+A^3BS^2)[(1-A^2)(1-A^3S^2)]^{-1}\\
&+(BT^2+B^2ST^3+ABST+ABT^2)[(1-A^2)(1-BT^2)]^{-1}\\
&+(BST^3+B^3S^2T^6)[(1-BT^2)(1-BST^3)]^{-1}\}. \qquad (3.1)
\end{aligned}
$$

The coefficient of $A^aB^bS^sT^t$ in the exansion of (3.1) is the multiplicity of the $SU(2)\times SU(2)$ representations (s,t) in the G_2 representation (a,b). The labels (s,t) are double the "angular momentum" labels.

The elementary multiplets implied by (3.1) are (10,11), (10,02), (20,00), (20,11), (30,20), (01,20), (01,02), (01,13), (02,00), (02,13), (11,11), (11,02), (21,11), (31,20). Combinations which are incompatible because of syzygies are the product of any two or the square of any one of (20,11), (21,11), (31,20), (02,13), (11,11), (11,02), and the products (20,00) (01,13), (30,20) (01,02), (30,20) (01,13), (30,20) (02,13), (30,20) (11,11), (30,20) (11,02), (01,02) (20,11), (01,02) (21,11), (01,02) (31,20), (01,13) (20,11), (01,13) (21,11), (01,13) (31,20), (01,13) (11,11), (01,13) (11,02). The notation is (ab,st).

IV. $G_2 \supset O(3)$ BRANCHING RULES

Racah[9] long ago pointed out the usefulness of the group G_2 in classifying many-particle states in the $l=3$ shell of atoms or nuclei. Since there are seven one-particle states, we are led to consider the chain $SU(7)\supset O(3)$. Since O(3) is not maximal in SU(7) but occurs in the chain $SU(7)\supset O(7)\supset G_2\supset O(3)$, one is forced to consider the reduction of G_2 representations according to O(3). Stone[7] has given an explicit formula for $G_2\supset O(3)$ branching rules, but since it contains plus and minus signs, with cancellations, it is not immediately useful for defining an integrity basis, or $G_2\supset O(3)$ polynomial bases.

The first step in obtaining a generating function for $G_2\supset O(3)$ branching rules is the conversion of the G_2 character generator into a generating function for O(3) weights contained in G_2 representations. The most convenient projection consists of the replacements $\eta\to x^{1/2}$, $\xi\to x^{3/2}$ (other substitutions, e.g., $\eta\to x^{5/2}$, $\xi\to x^{1/2}$, or $\eta\to x^2$, $\xi\to x$ are also possible). We obtain the generating function $H(A,B;x^{1/2},x^{3/2}) \equiv H(A,B;x)$, where x carries as its exponent the O(3) weight, or angular momentum projection. The second step consists of retaining only the part of $(1-x)H(A,B;x)$ whose expansion contains nonpositive powers of x. This result, with x^{-1} replaced by L, is the desired generating function.

Because all representations of G_2 are self-conjugate we have $H(A,B;x) = H(A,B;x^{-1})$. Also, from (2.7) we see that all terms in $H(A,B;x)$ contain the denominator factor $(1-Ax^3)(1-Ax^{-3})(1-Bx^5)(1-Bx^{-5})$. The latter property is the motivation for our choice of projection, since we expect $(1-AL^3)(1-BL^5)$ to be a common denominator factor in the final result.

We can exploit the properties of $H(A,B;x)$ discussed above to simplify the procedure. The symmetry of $H(A,B;x)$ under $x \leftrightarrow x^{-1}$ implies that the function $K(y) \equiv (1-y^2)H(A,B;y^2)/y$ is antisymmetric under $y \leftrightarrow y^{-1}$. Since $(1-AL^3)(1-BL^5)$ can appear as a denominator factor in the final generating function, we must be able to express $K(y)$ in the form

$$K(y) = \frac{P(y^{-1})}{(1-Ay^{-6})(1-By^{-10})} - \frac{P(y)}{(1-Ay^{6})(1-By^{10})}, \tag{4.1}$$

where the expansion of $P(y)$ contains only positive powers of y. The generating function we seek is just the first term on the right-hand side of (4.1), multiplied by y, and with the substitution of $y^{-2} \to L$.

Equation (4.1) can be rewritten as

$$\begin{aligned} P(y^{-1}) &= (1-Ay^{-6})(1-By^{-10})K(y) + P(y)(1-Ay^{-6}) \\ &\quad \times (1-By^{-10})[(1-Ay^{6})(1-By^{10})]^{-1} \\ &= (1-Ay^{-6})(1-By^{-10})K(y) \\ &\quad + P(y)[ABy^{-16} + (A^2B - B)y^{-10} \\ &\quad + (AB^2 - A)y^{-6} + (A^3B - AB)y^{-4} + \cdots]. \end{aligned} \tag{4.2}$$

In order to find $P(y^{-1})$ we need only keep powers of y^{-1} on the right-hand side. Terms in $P(y^{-1})$ of higher degree in y^{-1} than those from the second term in (4.2) are immediately determined from the first term. Lower degree terms can be found by solving a set of coupled algebraic equations.

The equations to be solved are

$$N_n = T_n + \sum_{k=0}^{8} f_k N_{k-n-1}, \tag{4.3}$$

where $N_i = 0$ for $i < 0$ and where

$$T(A,B;x^{-1}) = \tilde{T}(A,B;x^{-1}) + \sum_{k=0}^{7} T_k x^{-k} \tag{4.4}$$

```
M(A,B,L) = ((1-AL^3)(1-BL^5)(1-A^6))^-1
 x[AB^2L^6(1+A^3)(1+AL)(1+B)(1+B^5)(1+BL^4)(L^3+BL^2
  +B^2L+B^3)((1-B^2)(1-B^10)(1-A^2L^2)(1-B^2L^8))^-1

  +A^4L^6(1+A^3)(1+A^5)(1+AL)(1+AL^2)(1+A^3L)(1+AB)
  x((1-A^10)(1-A^2B^2)(1-A^2L^2)(1-A^2L^4))^-1

  +A^3L^6(1+A^3)(1+A^5)(1+AL^2)(1+AB)(1+BL)(1+A^3B+A^4B
  +A^3L+ABL+A^2BL)((1-A^10)(1-A^2B^2)(1-B^2L^2)(1-A^2L^4))^-1

  +(1+BL)(1+BL^4)((1+A^3)(1+B)(1+B^5)(B^4L^6+B^3L^7+B^2L^8
  +B^6L^9)+A(1+A^3)(1+B)(1+B^5)(B^2L^6+B^6L^7+B^5L^8+B^4L^9)
  +A^2(1+B)(1+B^5)(B^3L^6+B^2L^7+B^6L^8+B^5L^9)+A^5(B^11L^4+B^10L^5
  +(B^3+B^4+B^8+B^9)L^6+(B^2+B^3+B^7+B^8)L^7+(B^6+B^7+B^11)L^8
  +(B^5+B^6+B^10)L^9))((1-B^2)(1-B^10)(1-B^2L^2)(1-B^2L^8))^-1

  +ABL^5(1+A^3)(1+AL)(1+AB)(1+B)(1+B^5)
  x((1-B^2)(1-B^10)(1-A^2B^2)(1-A^2L^2))^-1

  +A^5L^5(1+A^3)(1+AL)(1+AB)(1+B)
  x((1-A^4)(1-B^2)(1-A^2B^2)(1-A^2L^2))^-1

  +A^4L^5(1+A^3)(1+A^5)(1+AL)(1+AB)(1+A^2+A^3)
  x((1-A^4)(1-A^10)(1-A^2B^2)(1-A^2L^2))^-1

  +B^4L^5(1+A^3)(1+AB)(1+B)(1+B^5)(1+BL)(B+A^2+A^2B^2)
  x((1-B^2)(1-B^10)(1-A^2B^2)(1-B^2L^2))^-1

  +AL^5(1+A^3)(1+A^5)(1+AB)(1+B^5)(1+BL)((B^3+B^5)
  +A(B+B^3+B^5)+A^2(B+B^3+B^4)+A^3(B+B^2+B^4)+A^4(1+B^2+B^4)+A^5B^2)
  x((1-A^10)(1-B^10)(1-A^2B^2)(1-B^2L^2))^-1

  +(1+BL)(L^5(1+A^3)(1+B^3)(1+B^5)(B^2+B^3+B^4+B^5+B^9)
  +AL^5(1+A^3)(1+B^3)(1+B^5)(B^3+2B^4+2B^5)+A^2L^5(1+B^3)(1+B^5)
  x(B^3+B^4+B^5+B^6+B^7)+A^5L^5(1+B^3)(B^4+B^5+2B^6+B^10+B^11+B^12)
  +A^5L^4(B^6+B^7+B^10+B^15)+A^5BL^3(1+B^15))
  x((1-B^2)(1-B^6)(1-B^10)(1-B^2L^2))^-1

  +[(1+A^15)(1+ABL^7)(1+A^5B^2)+(1+A^5)((1+ABL^7)(A^7+A^8)B
  +(1+ABL^5)((A^3+A^5+A^7)L+(1+A^2+A^3+A^4+A^5+A^7)BL+(A^2+2A^4)B^2L)
  +(1+ABL^3)((A^2+A^4+A^5+A^6+A^8)L^2+(A+A^2+2A^3+2A^4+2A^5+2A^6)BL^2
  +(A+A^2+2A^3+A^5)B^2L^2)+L^3((A^3+A^4+A^5+2A^6+A^9)+(A+2A^2+2A^3
  +2A^4+2A^5+2A^6+A^7)B+(A+2A^2+2A^3+A^4)B^2)+L^4((A^2+A^3+A^4+A^5
  +A^6+A^7)+(A^2+2A^3+3A^4+2A^5+2A^6+2A^7)B+(1+A+A^2+2A^3+A^4)B^2))]
  x((1-A^4)(1-A^10)(1-B^2)(1-A^2B^2))^-1

  +(1+A^5)[(1+ABL^7)((A^5+A^9)B+(A^4+A^7+A^8+A^11)B^2+(A+A^4+A^5+A^8)B^3
  +(A^3+A^6+A^7+A^10)B^4+(A^4+A^5+A^7+A^8)B^5+(A+A^4+A^7+A^10)B^6
  +(A^3+A^4+A^6+A^7)B^7+(A+A^4+A^5+A^8)B^8+(A^3+A^6+A^7+A^10)B^9
  +(1+A^3+A^4+A^7)B^10+(A^2+A^6)B^11)+L(1+B^5)(1+ABL^5)((A+A^3+2A^5
  +A^6+A^7+A^9)B^2+(A+A^2+2A^3+2A^4+2A^5+2A^6+A^7+A^8)B^3+(A+A^2+2A^3
  +2A^4+3A^5+A^6+A^7+A^8)B^4+(1+A+2A^2+2A^3+2A^4+2A^5+A^6+A^7)B^5
  +(1+A+2A^2+2A^3+3A^4+A^5+A^6+A^7)B^6+(A+A^2+A^3+2A^4)B^7)
  +L^2(1+B^5)(1+ABL^3)(A^7B+(1+A^2+A^3+3A^4+A^5+2A^6+A^7+A^8)B^2
  +(A+2A^2+2A^3+3A^4+4A^5+3A^6+2A^7+2A^8+A^9)B^3+(1+2A+2A^2+3A^3+4A^4
  +3A^5+2A^6+2A^7+A^8)B^4+(1+2A+3A^2+4A^3+4A^4+3A^5+2A^6+A^7)B^5
  +(1+2A+3A^2+3A^3+4A^4+3A^5+2A^6+A^8)B^6+(2A+2A^2+2A^3+A^4+2A^5)B^7)
  +L^3(1+B^5)(A^7+(A^4+A^8)B+(A^3+3A^4+3A^5+2A^6+2A^7+2A^8)B^2+(2+2A+2A^2
  +4A^3+4A^4+3A^5+2A^6+3A^7+A^8+A^9)B^3+(1+2A+4A^2+3A^3+4A^4+4A^5+3A^6
  +A^7+A^8+A^9)B^4+(1+3A+3A^2+4A^3+5A^4+3A^5+2A^6+A^7+A^8)B^5+(1+3A+3A^2
  +4A^3+4A^4+4A^5+2A^6+A^7)B^6+(2+3A+3A^2+2A^3+A^4)B^7)+L^4(1+B^5)
  x((A^5+A^6+A^7+A^8+A^9)B+(A+A^2+A^3+2A^4+2A^5+2A^6+A^7+A^8+A^9+A^10)B^2
  +(1+2A+3A^2+4A^3+4A^4+4A^5+3A^6+2A^7+A^8)B^3+(2+3A+3A^2+4A^3+5A^4
  +3A^5+A^6+2A^7+A^8)B^4+(1+3A+4A^2+4A^3+5A^4+4A^5+2A^6+A^7)B^5
  +(2+3A+4A^2+4A^3+4A^4+A^5+A^6)B^6+(2+2A+2A^2+3A^3+2A^4)B^7)]
  x((1-A^10)(1-B^2)(1-B^10)(1-A^2B^2))^-1

  +[(1+A^3)(1+ABL^7)((B^6+B^15)+A(B^9+B^11+B^12+B^14)+A^2(B^4+B^6
  +B^7+B^9)+A^3(B^3+B^12))+L(1+B^5)(1+ABL^5)((B^7+B^9+B^11)
  +A(B^8+B^9+B^10+B^11+B^12+B^13)+A^2(B^7+B^8+B^9+B^10+B^11+B^12)
  +A^3(B^8+B^9+B^10+B^11+B^12+B^13)+A^4(B^7+B^8+B^9+B^10+B^12)
  +A^5(B^6+B^7+B^8+B^9+B^10+B^11)+A^6(B^4+B^8+B^12))
  +L^2(1+B^5)(1+ABL^3)((2B^8+B^10+B^11+B^12)+A(B^7+2B^8+B^9+2B^10
  +2B^11+B^12+B^13)+A^2(2B^8+2B^9+B^10+2B^11+2B^12+B^13)+A^3(B^7+3B^8
  +B^9+B^10+3B^11+B^12)+A^4(B^7+2B^8+B^9+2B^10+2B^11+B^12+B^13)
  +A^5(B^5+B^6+B^7+2B^8+2B^9+B^10+B^11+B^12)+A^6(B^5+B^7+B^8+B^9+B^11))
  +L^3(1+B^5)((2B^9+B^10+B^11+B^12+2B^13)+A(2B^8+3B^9+B^10+3B^11
  +2B^12+2B^13)+A^2(2B^7+2B^8+B^9+3B^10+2B^11+B^12+B^13)+A^3(B^6+2B^7
  +B^8+3B^9+2B^10+B^11+2B^12)+A^4(B^5+B^7+3B^8+2B^9+B^10+2B^11+2B^12)
  +A^5(B^4+B^5+B^6+B^7+2B^8+B^9+2B^10+B^12+B^13)+A^6(2B^6+B^8+B^9+B^10))
  +L^4(1+B^5)((2B^8+B^9+2B^10+B^11+2B^12+B^13)+A(B^7+3B^8+2B^9+3B^10
  +2B^11+3B^12+B^13)+A^2(B^7+2B^8+2B^9+2B^10+2B^11+2B^12+B^13)
  +A^3(B^6+B^7+2B^8+2B^9+2B^10+2B^11+B^12+B^13)+A^4(2B^6+2B^7+2B^8+2B^9
  +2B^10+2B^11)+A^5(B^4+B^5+B^6+2B^7+B^8+2B^9+B^11)+A^6(B^5+B^7+B^9))]
  x((1-B^2)(1-B^6)(1-B^10)(1-A^2B^2))^-1]
```

FIG. 1. Generating function for $G_2 \supset O(3)$ branching rules.

is the part of $(1-x)H(A,B;x^{-1})$ which has nonpositive powers of x. The nonzero f_k are

$$f_2 = -AB(1-A^2), \quad f_3 = -A(1-B^2),$$
$$f_5 = -B(1-A^2), \quad f_8 = AB. \tag{4.5}$$

The final result for the desired generating functions is

$$M(A,B;L) = N(A,B;L)[(1-AL^3)(1-BL^5)]^{-1}, \tag{4.6}$$

where

$$N(A,B;x^{-1}) = \tilde{T}(A,B;x^{-1}) + \sum_{k=0}^{7} N_k x^{-k}. \tag{4.7}$$

This procedure considerably reduces the difficulty of the derivation, since the number of denominator factors we seek is reduced from eight to six. A further simplification was achieved by the independent determination of $M(A,B;0)$ by methods discussed in Sec. V.

The resulting generating function for $G_2 \supset O(3)$ branching rules appears as Fig. 1. This formula simplifies for some special cases. By setting $A = 0$, one obtains the generating functions for $G_2 \supset O(3)$ branching rules for $(0,b)$ representations of G_2:

$$\begin{aligned} M(0,B;L) = {} & [(1-B^2)(1-B^{10})(1-B^2L^2)(1-BL^5)]^{-1}\{(1+B)(1+BL)(1+BL^4) \\ & \times(B^2L^8 + B^3L^7 + B^4L^6 + B^5L^5 + B^6L^4 + B^7L^3 + B^8L^2 + B^9L)(1-B^2L^8)^{-1} \\ & + (1+BL)[(1+B^{15})(1+B^2L^5) + (B^2+B^3)(1+B^9)(L^4 + BL^3 + B^2L^2 + B^3L)](1-B^6)^{-1}\}. \end{aligned} \tag{4.8}$$

With $B = 0$, the $G_2 \supset O(3)$ generating function gives the O(3) content of $(a,0)$ representations of G_2, or $(a,0,0)$ representations of O(7); the formula has been presented elsewhere (see formula (31) of Ref. 6, and footnote 14 therein). Setting $L = 0$ in the $G_2 \supset O(3)$ generating function yields a generating function for O(3) scalars in G_2 representations. Its "substitution" into (4.9) of Ref. 10 would yield a generating function for O(3) scalars (including missing label operators) in the enveloping algebra of G_2.

V. CONCLUDING REMARKS

We mention here an alternative derivation. To obtain $G_2 \supset O(3)$ branching rules we could make use of the intermediate group $SU(2)\times SU(2)$ in the chain $G_2 \supset SU(2)\times SU(2) > O(3)$. Here O(3) is not a subgroup of $SU(2)\times SU(2)$ but is subjoined to it.[11] To derive the $SU(2)\times SU(2) > O(3)$ branching rules, it is necessary to triple the scale of weights of the second (i.e., T) SU(2) group [T generating function given by Eq. (3.1) of Ref. 11] and then to couple the two SU(2) representations by means of the SU(2) Clebsch–Gordan generating function.[1] The gererating function for $SU(2)\times SU(2) > O(3)$ branching rules is then

$$[(1-S^3T)(1-TL^{3/2})]^{-1}[(1-SL^{1/2})^{-1} + (1-TL^{1/2}ST + ST^2L^{1/2})(1-T^2)^{-1}]. \tag{5.1}$$

A complementary approach to the $G_2 \supset O(3)$ labelling problem would be to specify four missing label operators, O(3) scalars in the G_2 enveloping algebra. With J. Bystricky and J. Patera we plan to publish shortly a paper on this problem.

An obvious application of our G_2 character generator, Eq. (2.7) would be to derive a generating function for direct products of G_2 representations (the Clebsch–Gordan generating function).

ACKNOWLEDGMENT

We are grateful to J. Patera for assistance in the early stages of this work and for helpful discussions.

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The global symmetries of spin systems defined on abelian groups. I

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(Received 10 February 1981; accepted for publication 18 May 1981)

We consider the classification problem of the global symmetry groups of spin systems defined on abelian groups. Its implications on the generating functional, the transfer matrix, the Hamiltonian formalism, and factorization properties of spin systems are discussed. The duality properties of spin systems defined on semidirect products of abelian groups are revisited. In the first of this series of three papers we list the groups for systems defined on Z_p (p prime), $Z_2 \otimes Z_2$, and $Z_2 \otimes Z_2 \otimes Z_2$ manifolds. They are direct or wreath products of M-metacyclic groups and symmetric groups.

PACS numbers: 02.20.Km

1. INTRODUCTION

In the last few years there has been a flurry of work done in statistical mechanics on the phase structure of spin systems defined on abelian manifolds. They are generalized Ising (Z_2) models. This includes the Z_4, Z_5, Z_6, and Z_7 models,[1] the n-component Potts and vector Potts models (defined on Z_n),[2] and some models defined on $Z_m \otimes Z_n$ manifolds.[3] The interest in these models stems from their relevance to two-dimensional surface phenomena[4] and, possibly, to the understanding of confinement in particle physics.[5]

In this series of three papers we address the question of the global symmetries of spin systems defined on abelian manifolds. The knowledge of the global symmetry is important not only in order to find various symmetry relations among the observables of the system but it also helps to understand the nature of the phase transitions. All the systems mentioned before have built in a global invariance under the abelian group on which they have been defined. For example, a spin system defined on Z_7 has a Z_7 invariance, independent of which interaction we consider. For specific choices of the coupling constants, however, the symmetry is much larger. A known example is the case of the n-component Potts model which is defined on Z_n but has S_n (the group of all permutations of n objects) as global symmetry.[6]

We intend to study the problem in its full generality. We consider a spin system defined on an abelian group A (call it an *A system*) and look for all higher symmetries generated by special choices of the coupling constants.

We first remind the reader of the classification of the abelian groups and their irreducible representations. Next we formulate the problem of the classification of global symmetries and show several applications.

A. Abelian groups

The *abelian group A* is isomorphic to a direct product of cyclic groups[7]:

$$A = Z_{p_1^{m_1^{(1)}}} \otimes Z_{p_1^{m_1^{(2)}}} \otimes \cdots \otimes Z_{p_1^{m_1^{(j_1)}}} \otimes Z_{p_2^{m_2^{(1)}}} \otimes Z_{p_2^{m_2^{(2)}}} \otimes \cdots \otimes Z_{p_2^{m_2^{(j_2)}}} \otimes \cdots \otimes Z_{p_n^{m_n^{(1)}}} \otimes Z_{p_n^{m_n^{(2)}}} \otimes \cdots \otimes Z_{p_n^{m_n^{(j_n)}}}, \tag{1.1}$$

where $p_1, p_2, \ldots, p_n$ are prime numbers and $m_i^{(j)}$ are integers. In Eq. (1.1) Z_n denotes a cyclic group of order n. The order of the group A is $|A| = p_1^{m_1^{(1)} + \cdots + m_1^{(j_1)}} \cdots p_n^{m_n^{(1)} + \cdots + m_n^{(j_n)}}$. As an example we give the two abelian groups of order 12; they are $Z_2 \otimes Z_2 \otimes Z_3$ and $Z_4 \otimes Z_3 = Z_{12}$.

We label the group elements of the abelian group A using its cyclic subgroups. The n elements of a cyclic group Z_n can be labeled through an integer $\alpha (\alpha = 0,1,\ldots,n-1)$ with the multiplication rule

$$\alpha'' = \alpha + \alpha', \tag{1.2}$$

where the sum in Eq. (1.2) is done modulo n. The group elements of the direct product of two cyclic groups $Z_{n_1} \otimes Z_{n_2}$ are labeled by the double (α_1,α_2) with the group multiplication rule

$$(\alpha_1'',\alpha_2'') = (\alpha_1,\alpha_2) + (\alpha_1',\alpha_2'), \tag{1.3a}$$

$$\alpha_1'' = \alpha_1 + \alpha_1' (\text{mod } n_1),$$

$$\alpha_2'' = \alpha_2 + \alpha_2' (\text{mod } n_2). \tag{1.3b}$$

We denote the double (α_1,α_2) by $\hat{\alpha}$, where $\hat{\alpha}$ can be seen as a two component "vector", and write

$$\hat{\alpha}'' = \hat{\alpha} + \hat{\alpha}'. \tag{1.4}$$

This generalizes to any abelian group. Let us take, for example, the group $Z_2 \otimes Z_2 \otimes Z_3$. In this case

$$(\alpha_1'',\alpha_2'',\alpha_3'') = (\alpha_1,\alpha_2,\alpha_3) + (\alpha_1',\alpha_2',\alpha_3'). \tag{1.5}$$

Note that the operations for the first two components are done modulo 2 and for the last modulo 3.

The irreducible representations (which are one-dimensional and thus coincide with their characters) of an abelian group A are products of irreducible representations of its

 0022-2488/81/122740-13$01.00

cyclic components. The n irreducible representations of the cyclic group Z_n (group elements labeled by $\alpha \in Z_n$) are

$$\chi_r(\alpha) = \exp\left(\frac{2\pi i}{n} r\alpha\right), \tag{1.6}$$

where $r \in Z_n$. The irreducible representations of the group $Z_{n_1} \otimes Z_{n_2}$ are

$$\chi_{r_1,r_2}(\hat{\alpha}) = \exp\left(\frac{2\pi i}{n_1} r_1\alpha_1 + \frac{2\pi i}{n_2} r_2\alpha_2\right), \tag{1.7}$$

where $r_1, \alpha_1 \in Z_{n_1}$; $r_2, \alpha_2 \in Z_{n_2}$. We denote the irreducible representation (r_1,r_2) by $\hat{r}$. This generalizes to any abelian group. Returning to our example of the $Z_2 \otimes Z_2 \otimes Z_3$ group, its irreducible representations are labeled by

$$\hat{r} = (r_1,r_2,r_3) \tag{1.8}$$

and we have

$$\chi_{\hat{r}}(\hat{\alpha}) = (-1)^{r_1\alpha_1 + r_2\alpha_2} \exp\left(\frac{2\pi i}{3} r_3\alpha_3\right). \tag{1.9}$$

From now one we will denote the irreducible representations of the abelian group A (group elements labeled by $\hat{\alpha}$) by $\chi_{\hat{r}}(\hat{\alpha})$ ($\hat{r} = 0$ is the trivial representation).

B. Global symmetries

We are now in a position to *define our problem*. Consider a spin system defined on a lattice. In each lattice point P we define a variable $\hat{\alpha}$ which is an element of the abelian group A. The Lagrangian density

$$L = L(\hat{\alpha}_P - \hat{\alpha}_{P'}) \tag{1.10}$$

describes the interaction between the lattice points P and P'. Notice that L is defined on A, not on $A \otimes A$. In order to fix the ideas we assume that we have only interactions among nearest neighbors, although our considerations do not depend on this assumption. The action reads

$$S = \sum_{P,P' = n.n} L(\hat{\alpha}_P - \hat{\alpha}_{P'}), \tag{1.11}$$

where the sum is performed over the appropriate lattice points ($n.n$ = nearest neighbors).

The generating functional for the A system is

$$W = \sum_{\hat{\alpha}_P} \exp\left[-\beta S + \sum_P \sum_{\hat{r} \neq 0} J_{\hat{r},P}\chi_{\hat{r}}(\hat{\alpha}_P)\right]. \tag{1.12}$$

In Eq. (1.12) $\beta = 1/kT$ and $J_{\hat{r},P}$ represent the external sources. Taking derivatives with respect to the sources one obtains various corrrelation functions in the standard way. If in Eq. (1.12) the sources are taken independent of the lattice point P: $J_{\hat{r},P} = J_{\hat{r}}$ we obtain the partition function in the presence of $|A| - 1$ external fields. Taking the sources equal to zero in Eq. (1.12) one obtains the partition function of the system.

We now specify the Lagrangian density $L(\hat{\alpha})$. Two parametrizations are specially useful. One is the "*character*" *parametrization*

$$L(\hat{\alpha}) = \sum_{\hat{r} \in A} a_{\hat{r}}\chi_{\hat{r}}(\hat{\alpha}); \tag{1.13}$$

the other one is the "*orbit*" *parametrization*

$$L(\hat{\alpha}) = \sum_{\hat{\beta} \in A} b_{\hat{\beta}}\delta(\hat{\alpha} - \hat{\beta}). \tag{1.14}$$

In Eqs. (1.13) and (1.14) $a_{\hat{r}}$ and $b_{\hat{\beta}}$ are arbitrary coupling constants. Sometimes it is useful to use instead of the Lagrangian density the function

$$w(\hat{\alpha}) = \exp[-\beta L(\hat{\alpha})] \tag{1.15}$$

and to parametrize $w(\hat{\alpha})$ in terms of the characters

$$w(\hat{\alpha}) = \sum_{\hat{r} \in A} c_{\hat{r}}\chi_{\hat{r}}(\hat{\alpha}) \tag{1.16}$$

or, similar to (1.14),

$$w(\hat{\alpha}) = \sum_{\hat{\beta} \in A} d_{\hat{\beta}}\delta(\hat{\alpha} - \hat{\beta}). \tag{1.17}$$

The coefficients $d_{\hat{\beta}} = e^{-\beta b_{\hat{\beta}}}$ are called Boltzmann factors. The generating functional (1.12) is thus a function not only of the sources $J_{\hat{r},P}$ but also of the coupling constants.

In order to illustrate the two parametrizations (1.13) and (1.14) of the Lagrangian we give here the vector Potts model[2] in the character representation

$$L(\alpha) = 2\cos\left(\frac{2\pi}{n}\alpha\right) = \chi_1(\alpha) + \chi_{-1}(\alpha) \quad (\alpha \in Z_n) \tag{1.18}$$

and the n-component Potts model[2] in the orbit parametrization

$$L(\alpha) = \delta(\alpha) \quad (\alpha \in Z_n). \tag{1.19}$$

As in any physical problem one asks what are the symmetry properties of our system. The *global symmetry group* G is defined through the equation

$$L(g(\hat{\alpha}_P) - g(\hat{\alpha}_{P'})) = L(\hat{\alpha}_P - \hat{\alpha}_{P'}), \quad g \in G. \tag{1.20}$$

Here g is a one-to-one transformation which takes the "vector" $\hat{\alpha}$ into another vector $g(\hat{\alpha})$. This can also be seen as a permutation of the $|A|$ vectors $\hat{\alpha}$.

It is obvious that the transformations which satisfy (1.20) leave the action (1.11) invariant.

By construction, a system defined on an abelian group A has at least A itself as a global symmetry: the transformations ("translations") by $\hat{t}$,

$$\hat{\alpha}' = \hat{\alpha} + \hat{t}, \quad \hat{t} \in A, \tag{1.21}$$

obviously leave the action invariant. How can we have a higher symmetry in our problem? If there are relations among the coupling constants (there are fewer independent coupling constants than the order $|A|$ of the group). This can easily be seen in the "orbit" parametrization of L. Assume that G contains some permutation g which is not of the form (1.21). Then the global symmetry G induces by Eq. (1.20) a set of equalities $L(\hat{\alpha}_1) = L(\hat{\alpha}_2) = \ldots = L(\hat{\alpha}_s)$. $L(\hat{\alpha}_{s+1}) = \ldots = L(\hat{\alpha}_{s+r})$, etc. Equivalently $b_{\hat{\alpha}_1} = b_{\hat{\alpha}_2} = \ldots = b_{\hat{\alpha}_s}, b_{\hat{\alpha}_{s+1}} = \ldots = b_{\hat{\alpha}_{s+r}}$ etc. The converse is not true: not every set of equalities between the coupling constants $b_{\hat{\beta}}$ implies the existence of a symmetry larger than A. The equalities must be compatible with the group axioms of G (one can show that the existence of equalities for the constants $b_{\hat{\beta}}$ implies similar equalities—not other functional relations—for the constants $a_{\hat{r}}$).

As an example let us consider the implication of taking a "symmetric" Lagrangian (this choice is most often done in applications):

$$L(\hat{\alpha}_P - \hat{\alpha}_{P'}) = L(\hat{\alpha}_{P'} - \hat{\alpha}_P); (a_{\hat{r}} = a_{-\hat{r}}, b_{\hat{\beta}} = b_{-\hat{\beta}}). \tag{1.22}$$

The action S is invariant under the transformations

$$\hat{\alpha}' = \pm\hat{\alpha} + \hat{t}, \tag{1.23}$$

which form a non abelian group with $2|A|$ elements (with the exception of the $Z_2 \otimes \ldots \otimes Z_2$ case where $\hat{\alpha} = -\hat{\alpha}$).

To sum up, we address the following general question: for a given A system, which are *all* the global symmetry groups that can be obtained through special choices of the coupling constants? This is a formidable problem. We have restricted ourselves to the simplest cases in which A is one of the groups $Z_p, Z_p \otimes Z_{q'}, Z_{p^2}, Z_2 \otimes Z_2$, and $Z_2 \otimes Z_2 \otimes Z_2$ (p and q are prime numbers). For these special cases we are able to present a complete classification of the global symmetries. One gets non abelian groups with a very special structure: in most cases they are direct or wreath products of metacyclic and symmetric groups. Knowing this result one can choose a spin system with a given (nonabelian) global symmetry.

C. Physical applications

The control of the global symmetry of a spin system allows for various applications. We list some of them.

Kinematics. Let us take a symmetry G (this corresponds, for example, in the orbit parametrization of the Lagrangian to having fewer independent coupling constants: $\bar{b}_1 = b_{\hat{a}_1} = b_{\hat{a}_2} = \ldots = b_{\hat{a}_r}; \bar{b}_2 = b_{\hat{a}_{r+1}} = b_{\hat{a}_{r+2}} = \ldots = b_{\hat{a}_{2r}}; \ldots; \bar{b}_k = \ldots = \ldots = b_{|A|}$). The generating functional is a function of the sources and of the k-independent coupling constants:

$$W = W(\bar{a}_1, \bar{a}_2, \ldots, \bar{a}_k; J_{\hat{r},P}) = W(\bar{b}_1, \bar{b}_2, \ldots, \bar{b}_k; J_{\hat{r},P}). \tag{1.24}$$

The knowledge of the symmetry group gives in the usual way different symmetry relations of the function (1.24).

Hamiltonian (matrix formulation) of the theory. In order to find the properties of the A system one computes the spectrum of the transfer matrix. Its degeneracy is given by the dimensions of the irreducible representations of G. This is a problem on its own since for all the G groups appearing on the classification lists one has to determine the irreducible representations. As we shall see in Sec. 3 in some cases the answer is already known.

A place in which the importance of the global symmetries appears in a very striking way is the *Hamiltonian* formalism.[8] One considers a highly anisotropic 2-dimensional system corresponding to the continuous time-discrete space limit of the theory. In this limit the Hamiltonian is determined by the orbit structure of the Lagrangian, which in turn is specified by the global symmetry. It turns out that the Hamiltonian obtained this way is a special case of a more general class of Hamiltonians describing quantum systems having the same global symmetries as A systems.

This problem is presented in detail in Appendix A and several examples are given.

Factorization. Sometimes, from the knowledge of G, one can simplify the calculations of the generating functional. Let us consider two spin systems defined on two different abelian groups A and $\bar{A}$ of the same order (for example, $A = Z_{16}$ and $\bar{A} = Z_4 \otimes Z_4$). We assume that the global symmetry G is the same for the two systems. The two systems can then be mapped into each other. Consider the case in which $\bar{A} = A_1 \otimes A_2$. For special choices of the coupling constants the partition function of the $\bar{A}$ system factorizes into the product of the partition functions of the A_1 and A_2 systems. This property is easily seen in the $\bar{A}$ parametrization but would be very hard to observe in the A parametrization. Such a phenomenon is known to occur[9] in the Z_4 vector Potts model. In this case the factorization is seen immediately in the $Z_2 \otimes Z_2$ parametrization. We discuss this problem in Appendix B.

Phase transitions. Second order phase transitions are supposed to occur through the spontaneous breaking of the global symmetry.[10] The need for the knowledge of the possible global symmetries and their subgroups looks obvious. A fascinating problem occured to us when looking at the structure of the G groups which, as we mentioned before, is neat: Could one find a systematic connection between the critical exponents and the corresponding groups?

Duality. For two-dimensional systems defined on a square lattice with only nearest-neighbor interactions, it has been shown[11] that the partition function of an A system defined by the function $w(\hat{\alpha})$ given by Eq. (1.16) is equal up to a known factor to that of a system defined by a new function $\tilde{w}(\hat{\alpha})$:

$$\tilde{w}(\hat{\alpha}) = \frac{1}{|A|} \sum_{\hat{\gamma} \in A} w(\hat{\gamma}) \chi^*_{\hat{\alpha}}(\hat{\gamma}). \tag{1.25}$$

This is the Fourier transform of the original interaction.

As will be seen through different examples, if *the original system has a global symmetry G, the dual system has, in general, a global symmetry $\tilde{G}$ different from G* (in general the two groups do not even have the same order). The interplay of the two symmetries in the physical properties of the system is (to our knowledge) not yet understood.

A rather confusing situation exists in the literature about which spin systems in 2 dimensions admit a duality transformation and the current folklore is that the global symmetry has to be a semidirect product of abelian groups.[12] This is by no means true. Any A system admits a duality transformation and the global symmetry is not of this form in general. We discuss this problem in Appendix C.

D. Content of the papers

We have agonized a lot in order to find the most suitable way to present our results. We had to face the situation that a lot of the mathematics involved is unknown to physicists. We have thus decided to introduce it little by little and flood the text with examples. At the same time we have sent to the appendices the physical applications; not that we do not consider them very relevant but because we wanted to keep these papers in the spirit of a classification theory. Readers not interested in the mathematics but just in the results can pick them up in the right places.

This series of papers is organized as follows. We start with the present article. Here we confine ourselves mainly to the case when A is the cyclic group Z_p (p is a prime number).

All the global symmetries in this case are given by the M_p^k non abelian groups of order kp (k is a divisor of $p-1$). These groups consist of affine transformations with multiplications and additions done modulo p. These transformations are related to the automorphism group of Z_p and since the subject is in general unknown to physicists, in Sec. 2 we discuss the automorphism groups of abelian groups. The content of this section will be used not only in this paper but also in the succeeding ones.

In Sec. 3 we present in detail the global symmetries of spin systems defined on Z_p groups. We give the relations among the coupling constants and the symmetry properties of the generating functional.

In Sec. 4 we define the wreath product of finite groups. This type of product is again unknown to physicists but plays a crucial role in global symmetries.

In Sec. 5 we consider the $Z_2 \otimes Z_2$ case (this is the Ashkin–Teller problem[13]) and its generalization, which is the $Z_2 \otimes Z_2 \otimes Z_2$ problem. This case is not only interesting for possible applications but also because it shows a very special structure: all the relevant relations among the coupling constants are given by the automorphism group but the global symmetries are larger (they are written in terms of direct and wreath products).

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The Hamiltonian formalism for an A system and its connection with the orbit structure determined by the global symmetry is presented in Appendix A. The factorization of an A system into two subsystems is considered in Appendix B. The problems of systems defined on nonabelian manifolds is touched upon in Appendix C. It is shown that if the Lagrangian density is a class function defined on a group B which is the semidirect product of abelian groups the global symmetry is much larger than B. It can be found using the results known for A systems. Appendix D contains the group of automorphisms relevant to the $Z_2 \otimes Z_2 \otimes Z_2$ problem.

In paper II we consider the $Z_p \otimes Z_q$ (p and q are prime numbers) and the Z_{p^s} systems.

The first two papers do not contain proofs but just the proper definitions and results. The proofs are given in Paper III. Here we make use of chapters of group theory not yet used by physicists. We have tried to make the last paper self-contained although we expect only a few readers to go through it. A few results on the global symmetries of spin systems defined on non abelian manifolds are also presented in this paper. Some of the results presented in these papers are known in mathematics.[14] This refers to the classification of Z_p systems and to some properties of $Z_p \otimes Z_p$ systems. The others, as far as we know, are new.

2. THE AUTOMORPHISMS OP ABELIAN GROUPS. AFFINE GROUPS

It will be seen in the next sections that the group of automorphisms[15] of an abelian group A is an essential tool in finding the global symmetries.

Let $\hat{\alpha}_1, \hat{\alpha}_2 \in A$. An automorphism U is an invertible transformation obeying

$$U(\hat{\alpha}_1 + \hat{\alpha}_2) = U(\hat{\alpha}_1) + U(\hat{\alpha}_2). \tag{2.1}$$

We will often call U a "rotation."

Using the group law of A we can define the transformations

$$\hat{\alpha}' = \hat{\alpha} + \hat{t}, \quad \hat{t} \in A. \tag{2.2}$$

We will often call the transformation (2.2) a "translation" by $\hat{t}$. In group theory (2.2) is known as the regular representation of the abelian group A.

Combining Eqs. (2.2) and (2.3) we define the "*affine transformation*" $(U,\hat{t})$:

$$\hat{\alpha}' = (U,\hat{t})\hat{\alpha} = U(\hat{\alpha}) + \hat{t}. \tag{2.3}$$

We will denote the group of all automorphisms of A by H_A and the group of all affined transformations by $M_A^{H_A}$. The subgroups of $M_A^{H_A}$ obtained by taking affine transformations in which the rotations are various subgroups H of H_A will be denoted by M_A^H.

M_A^H is the semidirect product of A with H. It has, therefore, the order $|A||H|$ and it is nonabelian if $|H| > 1$.

In what follows we will be concerned with the case $A = Z_{p^s}$ (p = prime, s = integer), $A = Z_{p^s} \otimes \ldots \otimes Z_{p^s}$ and $A = Z_n$ (cases like $A = Z_{p^s} \otimes Z_{p^r}$, $r \neq s$, are more complicated).

A. The Z_{p^s} groups (p prime)

Let $\alpha \in Z_{p^s}$ be an integer modulo p^s. An automorphism U of Z_{p^s} is a multiplication of α by the integer u chosen such that p does not divide u (this guarantees the existence of an inverse) and $u < p^s$ (because we work modulo p^s):

$$U(\alpha) = u\alpha. \tag{2.4}$$

There are $p^s - p^{s-1}$ integers u. They form a group under multiplication modulo p^s. For $p \neq 2$ this group is cyclic: $H_{Z_{p^s}} = Z_{p^s - p^{s-1}}$. For $p = 2$, $s \geqslant 2$ the situation is different: $H_{Z_{2^s}} = Z_2 \otimes Z_{2^{s-2}}$.

The subgroups of H_A are easy to obtain: every subgroup of a cyclic group Z_n is a cyclic group Z_m with m dividing n. For each m there is a unique subgroup.

Thus (for $p \neq 2$) the group of affine transformations has the order $p^{2s-1}(p-1)$ and, to simplify the writing, we denote it by $M_{p^s}^{p^s - p^{s-1}}$. Taking subgroups of the automorphism group and combining them with the translations, we get the groups $M_{p^s}^k$ (k divides $p^s - p^{s-1}$). The affine transformations are thus

$$\alpha' = (v^m,t)\alpha = v^m\alpha + t. \tag{2.5}$$

Here $t = 0,1,...,p^s - 1$; $m = 0,1,...,k-1$ and v must be chosen such that k is the smallest positive integer for which $v^k = 1$. In Eq. (2.5) we have written u of Eq. (2.4) through a generator v of the subgroup Z_k.

A mnemonic rule for the group multiplication law is to write (v^m,t) as a matrix:

$$(v^m,t) = \begin{pmatrix} v^m & t \\ 0 & 1 \end{pmatrix}, \tag{2.6}$$

the multiplication rule being

$$\begin{pmatrix} v^m & t \\ 0 & 1 \end{pmatrix}\begin{pmatrix} v^{m'} & t' \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} v^{m+m'} & v^m t' + t \\ 0 & 1 \end{pmatrix}. \tag{2.7}$$

The groups $M^k_{p^s}$ are special cases of metacyclic groups. For the latter all irreducible representations and even the Clebsch–Gordan coefficients are known analytically.[16]

Let us give two examples. First take $A = Z_7$. In this case $H_{Z_7} = Z_6 = Z_2 \otimes Z_3$. The group of affine transformations is M^6_7 with the subgroups M^3_7 and M^2_7. It is important to know the values of v which enter in Eq. (2.5). For M^6_7, $v = 3$ or $v = 5$. For M^3_7, $v = 2$ or $v = 4$. For M^2_7, $v = 6$.

The second example is $A = Z_9$. $H_{Z_9} = Z_6$ and we obtain the groups M^6_9, M^3_9, and M^2_9. For M^6_9, $v = 2$ or $v = 5$. For M^3_9, $v = 4$ or $v = 7$. For M^2_9, $v = 8$.

Finally, note that there is no difficulty in getting a list of all M^H_A groups for $A = Z_{2^s}$.

B. The $Z_{p^s} \otimes \cdots \otimes Z_{p^s}$ (n times) groups

The group elements can be viewed as n-dimensional vectors:

$$\hat{\alpha} = (\alpha_1,\alpha_2,...,\alpha_n), \quad \alpha_1,\alpha_2,...,\alpha_n \in Z_{p^s} \tag{2.8}$$

(If $s = 1$ all the axioms of a vector space are satisfied!)

The automorphisms are given by all $n \times n$ invertible matrices U with entries in Z_{p^s}:

$$U(\hat{\alpha}) = \begin{pmatrix} u_{11} & \cdots & u_{1n} \\ \cdots & \cdots & \cdots \\ u_{n1} & \cdots & u_{nn} \end{pmatrix}\begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{pmatrix}. \tag{2.9}$$

The multiplication rule is that of usual matrices, but all operations are done modulo p^s. The invertibility condition is

$$\det U \neq 0, \quad \text{modulo } p \text{ (not } p^s). \tag{2.10}$$

We obtain groups of rather large order. For the case $s = 1$ the order of $H_{Z_p \otimes \cdots \otimes Z_p}$ is $(p^n - 1)(p^n - p)...(p^n - p^{n-1})$. This case is much studied in the context of discrete linear groups.[17]

As an example take $A = Z_2 \otimes Z_2$. The six automorphisms are

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}. \tag{2.11}$$

We leave the reader to check that this group is isomorphic to S_3.

C. The Z_n (n integer) group

We write the integer n as

$$n = p_1^{s_1} p_2^{s_2} \cdots p_m^{s_m}, \tag{2.12}$$

where $p_1,...,p_m$ are different prime numbers and $s_1,...,s_m$ are nonnegative integers. We have

$$Z_n = Z_{p_1^{s_1}} \otimes Z_{p_2^{s_2}} \otimes ... \otimes Z_{p_m^{s_m}}. \tag{2.13}$$

It is easy to see that the affine group factorizes:

$$M^{H_{Z_n}}_{Z_n} = \bigotimes_{i=1}^{m} M^{H_{Z_{p_i^{s_i}}}}_{Z_{p_i^{s_i}}}. \tag{2.14}$$

Take $n = pq$ (p and q primes) as an example. In this case $\hat{\alpha}$ has two components: $\hat{\alpha} = (\alpha_1,\alpha_2)$ with $\alpha_1 \in Z_p$ and $\alpha_2 \in Z_q$. The affine transformations are [compare with Eq. (2.5)]

$$\alpha_1' = u_1^{m_1}\alpha_1 + t_1 (\text{mod } p) \quad \alpha_2' = v_2^{m_2}\alpha_2 + t_2 (\text{mod } q). \tag{2.15}$$

THE GLOBAL SYMMETRIES OF Z_p SYSTEMS (p PRIME)

The case where the abelian manifold is Z_p (p prime) is by far the simplest one. The Lagrangian density [see Eqs. (1.13) and (1.14)] reads

$$\begin{aligned} L(\alpha_P - \alpha_{P'}) &= \sum_{r=0}^{p-1} a_r \exp\left[\frac{2\pi i}{p} r(\alpha_P - \alpha_{P'})\right] \\ &= \sum_{\beta=0}^{p-1} b_\beta \delta(\alpha_P - \alpha_{P'} - \beta) \end{aligned} \tag{3.1}$$

$$(\alpha_P,\alpha_{P'}, \beta \in Z_p).$$

We look for all possible global symmetry groups G.

$$L(g(\alpha_P) - g(\alpha_{P'})) = L(\alpha_P - \alpha_{P'}), \quad g \in G. \tag{3.2}$$

At this point we can clarify why we have coined the name *orbit* to the parametrization b_β in Eq. (3.1). The concept "orbit" is crucial in our discussion. We thought it useful to introduce it here in order to familiarize the reader with it.

Consider a function of two variables $L(\alpha_P,\alpha_{P'})$ and let $g \in G$ be a symmetry transformation of L:

$$L(g(\alpha_P),g(\alpha_{P'})) = L(\alpha_P,\alpha_{P'}). \tag{3.3}$$

Take a pair $(\alpha^1_P,\alpha^1_{P'})$ and consider the pairs $(g(\alpha^1_P), g(\alpha^1_{P'}))$ for all $g \in G$. The resulting set of pairs is called an *orbit* of G in the set of all possible pairs. We label it by θ_1. Repeat now the operation with another pair $(\alpha^2_P,\alpha^2_{P'})$ not contained in θ_1. The result is an orbit θ_2 disjoint from θ_1. Repeat the operation again up to the exhaustion of all possible pairs. *The global symmetry condition* (3.3) *means that L is constant on each orbit.*

We now return to our Z_p invariant Lagrangian (3.1). If the global symmetry is not larger than the built-in Z_p symmetry ($G = Z_p$) the orbits θ_β are given by the sets of pairs $(\alpha_P,\alpha_{P'})$ satisfying

$$\alpha_P = \alpha_{P'} + \beta. \tag{3.4}$$

The value of L on θ_β is b_β. If G is larger than Z_p the orbits will be reunions of θ_β.

Let v be the generator of the subgroup Z_k of the automorphism group of Z_p [see Eq. (2.5) for $s = 1$]. Assume $v \in G$. Then, by Eqs. (3.2), (2.4), and (2.5)

$$L(u\alpha) = L(v^m\alpha) = L(\alpha). \tag{3.5}$$

This implies, by Eq. (3.1),

$$a_r = a_{vr} = a_{v^2r} = \cdots = a_{v^{k-1}r}, \tag{3.6a}$$

$$b_\beta = b_{v\beta} = b_{v^2\beta} = \cdots = b_{v^{k-1}\beta}, \tag{3.6b}$$

together with identical relations for the c_r and d_s coefficients from Eqs. (1.15) and (1.16). In other words, all the pairs $(\alpha_P,\alpha_{P'})$ obeying

$$\alpha_P = \alpha_{P'} + v^m\beta, \quad m = 0,\ 1,...,k-1 \tag{3.7}$$

belong to the same orbit.

In this way we have shown that the affine transformations

$$\alpha' = v^m\alpha + t, \quad m \in Z_k,\ t \in Z_p \tag{3.8}$$

obtained by combining Z_k "rotations" with Z_p "translations", are symmetries of the Lagrangian (3.1). If $k \neq p-1$ they are the only symmetry transformations consistent with (3.6) and G is the M_p^k group introduced in Sec. 2.

If $k = p-1$, G contains the whole automorphism group of Z_p. In this case Eq. (3.6) reads

$$a_1 = a_2 = ... = a_{p-1};\quad b_1 = b_2 = ... = b_{p-1} \tag{3.9}$$

and the Lagrangian has the expression

$$L(\alpha_P - \alpha_{P'}) = a_0 - a_1 + pa_1\delta(\alpha_P - \alpha_{P'}). \tag{3.10}$$

This function is obviously invariant under any permutation g of the p values of α. Thus the maximal symmetry is S_p (the symmetric group of p objects).

We summarize the situation as follows.

Theorem: Each possible global symmetry of a Z_p-system is determined by a subgroup Z_k (k is a divisor of $p-1$) of the automorphism group Z_{p-1}. The relations among the coupling constants are given by Eq. (3.6). If $k \neq p-1$ the maximal global symmetry is the nonabelian group M_p^k of the affine transformations (3.8). This group is of order pk. If we take the whole automorphism group Z_{p-1}, the relations among the coupling constants particularize to (3.9) and the maximal global symmetry is S_p.

The proof of this theorem goes back to Burnside's work done in 1901 (!)[18] and will be given for completeness in paper III.

We exemplify the theorem with the Z_7 system considered in Sec. 2. The automorphism group is $Z_6 = Z_2 \otimes Z_3$. There are three possible symmetry groups larger than Z_p itself (all the operations are done modulo 7):

(a) M_7^2 with the group elements

$$\alpha' = \pm\alpha + t, \quad \alpha,\ t \in Z_7. \tag{3.11a}$$

This implies

$$a_1 = a_6,\ a_2 = a_5,\ a_3 = a_4. \tag{3.11b}$$

(b) M_7^3 with

$$\alpha' = 2^m\alpha + t, \quad m = 0,1,2, \tag{3.12a}$$

$$a_1 = a_2 = a_4,\ a_3 = a_5 = a_6. \tag{3.12b}$$

(c) S_7 for which the relations among the coupling constants,

$$a_1 = a_2 = a_3 = a_4 = a_5 = a_6, \tag{3.13}$$

are already generated by M_7^6 but they admit as symmetry transformations all perturbations of 7 objects.

Let us make some comments. The very simple structure described by the theorem does not generalize to other A systems. The subgroups of the automorphism group of A will always play a crucial role in the classification problem, but

(i) They do not always generate all possible symmetries of the Lagrangian.

(ii) There are cases where the relations among the coupling constants are indeed generated by a subgroup of the automorphism group but the maximal symmetry group is larger than the corresponding affine group.

(iii) A subgroup of the automorphism group may sometimes generate the same relations as one of its own subgroups.

We turn now to the duality transformation (1.25). We consider a Z_p system with the global symmetry M_p^k [the coupling constants verify Eq. (3.6)] and look for the global symmetry of the Fourier transformed system.

We write the function $w(\alpha)$ in the character parametrization:

$$w(\alpha) = \sum_{r=0}^{p-1} c_r\chi_r(\alpha). \tag{3.14}$$

The M_p^k symmetry implies

$$c_r = c_{vr} = \cdots = c_{v^{k-1}r}, \tag{3.15a}$$

$$d_\beta = d_{v\beta} = \cdots = d_{v^{k-1}\beta}. \tag{3.15b}$$

The Fourier transform of $w(\alpha)$ is

$$\tilde{w}(\alpha) = \sum_{r=0}^{p-1} c_r\delta(\alpha - r). \tag{3.16}$$

From Eq. (3.16) we see that the coupling constants in the character representation of $w(\alpha)$ are also the coupling constants in the orbit parametrization of $\tilde{w}(\alpha)$ (and vice versa). Thus Eq. (3.15) implies that the $\tilde{w}$ system has also M_p^k as a global symmetry.

In conclusion: for Z_p systems the orginal system and its dual have the same global symmetry. For other A systems this may not be the case. This stems from the fact that unlike (3.15) the relations among the c_r coefficients and those among the d_β coefficients are in general different.

We now consider the consequences of global symmetries on the generating functional defined by Eq. (1.12). We have

$$W(c_s;\ J_{P,r}) = \sum_{\alpha_P} \prod_{\text{n.n.}} \Big(\sum_{s=0}^{p-1} c_s\chi_s(\alpha_P - \alpha_{P'})\Big) \times \exp\Big[\sum_P \sum_{r=1}^{p-1} J_{P,r}\chi_r(\alpha_P)\Big], \tag{3.17a}$$

$$W(d_\beta;\ J_{P,r}) = \sum_{\alpha_P} \prod_{\text{n.n.}} \Big(\sum_{\beta=0}^{p-1} d_\beta\delta(\alpha_P - \alpha_{P'} - \beta)\Big) \times \exp\Big[\sum_P \sum_{r=1}^{p-1} J_{P,r}\chi_r(\alpha_P)\Big]. \tag{3.17b}$$

Consider the change of variables given by the affine transformations $\alpha' = u\alpha + t\,(u,t \in Z_p)$. Without any assumption on c_s and d_β we get

$$W(c_s;\ J_{P,r}) = W(c_{us};\ \chi_{ur}(t)\,J_{P,ur}), \tag{3.18a}$$

$$W(d_\beta;\ J_{P,r}) = W(d_{u^{-1}\beta};\ \chi_{ur}(t)\,J_{P,ur}), \tag{3.18b}$$

where

$$u = 1,2,...,p-1; \quad t = 0,1,2,...,p-1. \tag{3.18c}$$

This equation is the most general kinematical consequence of the fact that the Z_p symmetry is built-in by writing the interaction as a function of $\alpha_P - \alpha_{P'}$. A more general change of variables does not preserve this property. In Eq. (3.18), the $J_{P,r}$ transform according to the only $(p-1)$-dimensional representation of M_p^{p-1}.[16]

If the global symmetry group is M_p^k rather than Z_p Eq. (3.18) holds, but there are fewer independent coupling constants according to Eq. (3.6). An important special case of Eq. (3.18) is then $u = v^m \in Z_k$, because the coupling constants remain unchanged:

$$W(c_s;\ J_{P,r}) = W(c_s;\ \chi_{v^m r}(t)J_{P,v^m r}), \tag{3.19a}$$

$$W(d_\beta;\ J_{P,r}) = W(d_\beta;\ \chi_{v^m r}(t)J_{P,v^m r}). \tag{3.19b}$$

Equations (3.18) and (3.19) hold if instead of c_s and d_β we use the coupling constants of the Lagrangian a_s respectively b_β.

As an example we consider again the Z_7 systems. We choose M_7^2 as a global symmetry and [see Eq. (3.15b)], d_1,d_2,d_3 as independent couplings. From Eq. (3.18b) we get, with $u = 2,3,4,5$,

$$\begin{aligned} &W(d_1,d_2,d_3;\ J_{P,r}) \\ &\quad = W(d_3,d_1,d_2;\ e^{(4\pi i/7)rt}J_{P,2r}) \\ &\quad = W(d_2,d_3,d_1;\ e^{(6\pi i/7)rt}J_{P,3r}) \\ &\quad = W(d_2,d_3,d_1;\ e^{(8\pi i/7)rt}J_{P,4r} \\ &\quad = W(d_3,d_1,d_2;\ e^{(10\pi i/7)rt}J_{P,5r}), \end{aligned} \tag{3.20}$$

and from Eq. (3.19b) with $v = 6$ and $m = 0$ and 1,

$$\begin{aligned} &W(d_1,d_2,d_3;\ J_{P,r}) \\ &\quad = W(d_1,d_2,d_3;\ e^{(\pm 2\pi i/7)rt}J_{P,\pm r}). \end{aligned} \tag{3.21}$$

A pathological case occurs when the global symmetry is S_p [see Eqs. (3.9) and (3.10)]. In this case we have only one independent coupling constant and we get

$$W(d_1;\ J_{P,r}) = W(d_1;\ J^g_{P,r}), \quad g \in S_p \tag{3.22}$$

where the new sources $J^g_{P,r}$ are determined by the equations

$$\sum_{r=0}^{p-1} J^g_{P,r}\chi_r(\alpha) = \sum_{r=0}^{p-1} J_{P,r}\chi_r(g(\alpha)). \tag{3.23}$$

Here g is any element of the symmetric group S_p. Equation (3.23) shows that the sources behave like a $(p-1)$-dimensional representation of the group S_p.

4. WREATH PRODUCTS

In physics we got used to the notation of direct product of groups. It is to our knowledge for the first time that another type of product, the *wreath product*,[7,15,17] is proven a very useful device. We define it here and show some applications in the next section.

We consider two groups G and H of order $|G|$ and $|H|$ and write the direct product of n copies of G and H:

$$G \otimes G \otimes \cdots \otimes G \otimes H. \tag{4.1}$$

This is a group order $|G|^n|H|$. One can, however, define another product of the same n copies of G and H. This can be done if G is a subgroup of S_m (the group of all permutations of m objects) and H is a subgroup of S_n (same n as the number of copies). G is called a permutation group of degree m, H is then a permutation group of degree n. G has an m-dimensional representation in which every $g \in G$ acts as a permutation of the basis vectors e_μ:

$$ge_\mu = e_{g(\mu)}, \quad \mu = 0,1,..,m-1,\ g \in G. \tag{4.2}$$

$g(\mu)$ shows how the indices are permuted. Similarly

$$hf_\nu = f_{h(\nu)}, \quad \nu = 0,1,...,n-1,\ h \in H. \tag{4.3}$$

Now we take n copies of G (n is the degree of H!) and one copy of H. We can define a new group by making H act on the elements of $G \otimes G \otimes \cdot \otimes G$ (n times). The new group is called the wreath product of G with H and is denoted by $G \wr H$.

It is convenient to define the group $G \wr H$ through its action on its $n \cdot m$ dimensional representation. We denote the basis vectors of this representation by $e_{\mu,\nu}$ ($\mu = 1,...m$, $\nu = 1,...n$) and an element of $G \wr H$ by $(g_0,g_1,...,g_{n-1};h)$. We have by definition

$$(g_0,g_1,...,g_{n-1};\ h)e_{\mu,\nu} = e_{g_\nu(\mu),h(\nu)}. \tag{4.4}$$

If we look at the objects $e_{\mu,\nu}$ as the elements of an $m \times n$ matrix, g_0 acts on the first line, g_1 on the second, etc., h permutes the lines. $G \wr H$ has the order $|G|^n|H|$.

The group multiplication law is easily deduced from Eq. (4.4):

$$\begin{aligned} &(g_0,g_1,...,g_{n-1};\ h)(g'_0,g'_1,...,g'_{n-1};\ h')e_{\mu,\nu} \\ &\quad = (g_0,g_1,...,g_{n-1};\ h)e_{g'_\nu(\mu),h'(\nu)} \\ &\quad = e_{g_{h'(\nu)}(g'_\nu(\mu)),hh'(\nu)} \end{aligned} \tag{4.5}$$

or

$$\begin{aligned} &(g_0,g_1,...,g_{n-1};\ h)(g'_0,g'_1,...,g'_{n-1};\ h') \\ &\quad = (g_{h'(0)}g'_0,g_{h'(1)}g'_1,...,g_{h'(n-1)}\cdots g'_{n-1};\ hh'). \end{aligned} \tag{4.6}$$

From Eq. (4.6) one notices that $G \wr H$ is the semidirect product of $G \otimes \cdots \otimes G$ (the normal subgroup) with H.

An important property of the wreath product is its associativity:

$$(G \wr H) \wr K = G \wr (H \wr K) = G \wr H \wr K. \tag{4.7}$$

It is important to note that the definition of the wreath product $G \wr H$ takes two permutation groups ($G \subset S_m$, $H \subset S_n$) into another permutation group ($G \wr H \subset S_{mn}$). It is this point of view which is used in looking for global symmetries.

We now consider as an example the $Z_2 \wr Z_2$ group which is of order 8. In this case we have

$$\begin{aligned} &g_\alpha e_\mu = e_{\alpha+\mu};\ h_\beta\ f_\nu = f_{\beta+\nu} \\ &\quad (\alpha,\beta,\mu,\nu \in Z_2) \end{aligned} \tag{4.8}$$

A group element of $Z_2 \wr Z_2$ can be labeled as $(\alpha_0,\alpha_1;\beta)$ and its action on $e_{\mu,\nu}$ reads

$$(\alpha_0,\alpha_1;\ \beta)e_{\mu,\nu} = e_{\alpha_\nu+\mu,\beta+\nu}. \tag{4.9}$$

The group multiplication rule is

$$(\alpha_0,\alpha_1;\ \beta)(\alpha'_0,\alpha'_1;\ \beta') = (\alpha_{\beta'}+\alpha'_0,\alpha_{\beta'+1}+\alpha'_1;\ \beta+\beta'). \tag{4.10}$$

It is trivial to check that Eq. (4.10) corresponds to the dihedral group D_4.

5. THE $Z_2 \otimes Z_2$ AND $Z_2 \otimes Z_2 \otimes Z_2$ SYSTEMS

We consider the generating functional (1.12) and the Lagrangian (1.10) to (1.11) in the case where the vectors $\hat{\alpha}, \hat{\beta}$, and $\hat{r}$ have n components taking values in Z_2. The $n = 2$ case corresponds to the well-known $Z_2 \otimes Z_2$ Ashkin–Teller model.[13] For $n = 3$ one gets the $Z_2 \otimes Z_2 \otimes Z_2$ model which to our knowledge has not yet been studied. We will not consider here higher values of n.

We now write the symmetry relations for the generating functional [the analog of Eqs. (3.18) in the Z_p case]. We consider the change of variables given by an affine transformation

$$\hat{\alpha}' = U\hat{\alpha} + \hat{t}, \tag{5.1}$$

where U is an invertible $n \times n$ matrix with entries in Z_2 and $\hat{t} \in Z_2 \otimes Z_2 \otimes Z_2$. We have

$$W(c_{\hat{s}};\ J_{P,\hat{r}}) = W(c_{U^T\hat{s}};\ \chi_{U^T\hat{r}}(\hat{t})J_{P,U^T\hat{r}}), \tag{5.2a}$$

$$W(d_{\hat{\beta}};\ J_{P,\hat{r}}) = W(d_{U^{-1}\hat{\beta}};\ \chi_{U^T\hat{r}}(t)J_{P,U^T\hat{r}}). \tag{5.2b}$$

The same relations hold if instead of $c_{\hat{s}}$ and $d_{\hat{\beta}}$ one writes $a_{\hat{s}}$ and $b_{\hat{\beta}}$. In Eqs. (5.2) U^T is the transpose of the matrix U. Keeping in mind that the automorphism group has 6 elements in the $Z_2 \otimes Z_2$ case and 168 elements in the $Z_2 \otimes Z_2 \otimes Z_2$ case (see Sec. 2), we get 24 respectively 1344 symmetry relations.

If we require the action to be invariant under an affine transformation (5.1) one obtains the following constraints on the coupling constants:

$$a_{\hat{r}} = a_{U^T\hat{r}}, \quad b_{\hat{\beta}} = b_{U\hat{\beta}}. \tag{5.3}$$

Notice that the relations among the coupling constants in the character and orbit parametrizations are in general different [as opposed to the Z_p case, see Eq. (3.6)].

Since the global symmetries are only affine transformations in the $Z_2 \otimes Z_2$ case but not for $Z_2 \otimes Z_2 \otimes Z_2$, we consider the two cases separately.

A. The $Z_2 \otimes Z_2$ problem

As seen in Sec. 2 the automorphism group is S_3 in this case. The six group elements given by Eq. (2.11) can be separated in three classes:

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{5.3a}$$

$$U_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, U_2 = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}, U_3 = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}, \tag{5.3b}$$

$$U_4 = \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix}, U_4^2 = \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix}. \tag{5.3c}$$

The group elements in the class (5.3b) are of order two and those in the class (5.3c) are of order three.

Using the notations introduced in Sec. 2, the group of all affine transformations is $M^{S_3}_{Z_2 \otimes Z_2}$. This group has 24 elements and is isomorphic to S_4. It has three subgroups $M^{Z_2}_{Z_2 \otimes Z_2}$ [given by the three U_i of Eq. (5.3b)] and one subgroup $M^{Z_3}_{Z_2 \otimes Z_2}$ (given by the two automorphisms of order three). One notices that $M^{Z_2}_{Z_2 \otimes Z_2}$ is isomorphic to $Z_2 \wr Z_2$. The relations among the coupling constants corresponding to these subgroups are derived using Eq. (5.3). We obtain

$$(U_1) \quad a_{1,0} = a_{0,1}, \quad b_{1,0} = b_{0,1}, \tag{5.4a}$$

$$(U_2) \quad a_{0,1} = a_{1,1}, \quad b_{1,0} = b_{1,1}, \tag{5.4b}$$

$$(U_3) \quad a_{1,0} = a_{1,1}, \quad b_{0,1} = b_{1,1}, \tag{5.4c}$$

for the $Z_2 \wr Z_2$ subgroups and

$$(U_4) \quad a_{1,0} = a_{0,1} = a_{1,1}, \quad b_{1,0} = b_{0,1} = b_{1,1} \tag{5.5}$$

for the $M^{Z_3}_{Z_2 \otimes Z_2}$ group. We notice that Eq. (5.5) implies already S_4 as a global symmetry.

One can check that there are no other symmetry relations than those given by affine transformations. To sum up, the global symmetries of a $Z_2 \otimes Z_2$ system are

$$\begin{aligned} &(1) \quad Z_2 \otimes Z_2 \quad \text{(arbitrary coupling constants)}, \\ &(2) \quad Z_2 \wr Z_2 \quad \text{[Eqs. (5.4a)–(5.4c)]}, \\ &(3) \quad S_4 \quad \text{[Eqs. (5.5)]}. \end{aligned} \tag{5.6}$$

It is interesting to notice an important difference between the structure of the global symmetries of a $Z_2 \otimes Z_2$ system and of a Z_p system. Although the symmetries are given by subgroups of affine transformations the global symmetry might be larger. This is the case for the $M^{Z_2}_{Z_2 \otimes Z_2}$ subgroup when the global symmetry is S_4.

The symmetry relations for the generating functional can be derived using Eqs. (5.2) and (5.3). In particular one recovers the known result[13] that the partition function is invariant under a permutation of the three coupling constants. This is a consequence of the automorphism group being S_3.

Finally, from Eqs. (5.4) and (5.5) we conclude that if a system has one of the symmetries (5.6), its dual has the same symmetry.

B. The $Z_2 \otimes Z_2 \otimes Z_2$ case

We first derive the relations among the coupling constants corresponding to the invariance under affine transformations. The automorphism group $H_{Z_2 \otimes Z_2 \otimes Z_2}$ consists (see Sec. 2) of all invertible 3×3 matrices with entries in Z_2. One gets a group of order 168 with 21 elements of order 2, 56 of order 3, 42 of order 4, and 48 of order 7. Since these matrices are necessary in order to apply Eqs. (5.2), they are given in Appendix D.

The symmetry relations for the coupling constants derived taking various subgroups of $H_{Z_2 \otimes Z_2 \otimes Z_2}$ are displayed in Table I. For each type of symmetry there are several equivalent ones which correspond to different choices of the basis [similar to Eqs. (5.4a)–(5.4c) in the $Z_2 \otimes Z_2$ case]. For example, there are 7 equivalent relations for the symmetry (d), 21 for the symmetry (e), etc. In order to obtain them all one has to do the following substitutions in Table I:

$$a_{\hat{\alpha}} \to a_{V\hat{\alpha}}. \tag{5.7}$$

Here the transformations V are C^l ($l = 0, 1 \ldots 6$) for the case when we have 7 equivalent relations, $C^l A^m$ ($m = 0, 1, 2$) when we have 21 relations, and $C^l B^n$ ($n = 0, 1, 2, 3$) in the case of 28 relations. The matrices A, B, and C are given in Appendix D.

There are many new features which we have learned in deriving the results shown in Table I.

(1) Taking a subgroup of $H_{Z_2\otimes Z_2\otimes Z_2}$ and deriving the relations among the coupling constants, one observes that the Lagrangian may be automatically invariant under a larger subgroup. If one asks, for example, a Z_3 invariance one gets $S_3 \subset H_{Z_2\otimes Z_2\otimes Z_2}$ invariance [see symmetry (f)].

(2) All possible symmetry relations among the coupling constants can be obtained considering affine transformations but, with the exception of the (a), (b), and (f) cases, the global symmetries are actually larger. We have determined them using the methods presented in Paper III and give them here without proof. Consider, for example, the (c) case. Here the subgroup of affine transformations is of order 32 but the global symmetry $Z_2 \wr (Z_2 \otimes Z_2)$ is of order 64. One notices that the global symmetries have a very simple structure. They are direct or wreath products of Z_2 and S_4.

(3) One notices that for the (c) and (d) respectively (g) and (h) symmetries the relations among the couplings in the character and orbit parametrizations are interchanged. That means [see Eqs. (1.25), (3.14), and (3.16)] that if a spin system has the global symmetry (c) its dual has the symmetry (d) (and vice versa). Similarly, if the system has the symmetry (g) its dual has the symmetry (h) (and vice versa). Notice that the order of the groups entering each couple is different: 32 and 64 respectively 384 and 1152. An easy way to remember this phenomenon is to notice that if a system has the symmetry $G \wr H$ its dual has the symmetry $H \wr G$.

We now turn to the problem of the symmetry relations for the generating functional in the case in which the system has a global symmetry larger than a subgroup of affine transformations [this is similar to the S_p global symmetry for Z_p systems when the symmetry relations are given by Eq. (3.22)]. As an example let us assume that the coupling constants satisfy the conditions for case (h). In this case, together with the changes of variables given by affine transformations [see Eqs. (5.2)] (there are 1344), one has to consider the changes of variables given by those elements of the group $S_4 \wr Z_2$ of order 1152 which are not affine transformations. One generates in this way a larger group of order 8064 and one can write the corresponding symmetry relations (the figure 8064 is derived observing that neither the affine transformations nor $S_4 \wr Z_2$ have elements of order 5 and that $|S_8|_{/5} = 8!/_5 = 8064$ is the smallest number having both 1152 and 1344 as divisors). We did not take the pain to study this group, neither did we look for the corresponding groups for other cases.

ACKNOWLEDGMENTS

This work was started during the visit by one of us (V. R.) at the Weizmann Institute. V. R. would like to thank his colleagues there for their kind hospitality and useful discussions. We are also grateful to Stuart Samuel for his interesting observations.

APPENDIX A: THE HAMILTONIAN FORMALISM FOR AN A SYSTEM

In this appendix we give the Hamiltonian formalism[8] for an A system. We consider a 2-dimensional square lattice with the lattice points labeled by the double (s,μ). Here $s = 1,2,\ldots,M$ labels the lines and $\mu = 1,2,\ldots,M$ the columns. The partition function for the system is

$$W = \sum_{\hat{\alpha}_\mu^s} \exp\left\{ -\sum_{\mu=1}^{M} \left[\xi_C C(\hat{\alpha}_\mu^s, \hat{\alpha}_{\mu+1}^s) + \xi_D D(\hat{\alpha}_\mu^s)\right]\right\}, \quad \text{(A1)}$$

where

$$C(\hat{\alpha}_\mu^s, \hat{\alpha}_{\mu+1}^s) = \sum_{s=1}^{M} L(\hat{\alpha}_\mu^s - \hat{\alpha}_{\mu+1}^s), \quad (\hat{\alpha}_\mu^s \in A). \text{(A2)}$$

$$D(\hat{\alpha}_\mu^s) = \sum_{s=1}^{M} L(\hat{\alpha}_\mu^s - \hat{\alpha}_\mu^{s+1}),$$

In Eq. (A1) we assume that the interactions along the columns and the lines have different strengths $(\xi_C \neq \xi_D)$.

TABLE I. The global symmetries of $Z_2 \otimes Z_2 \otimes Z_2$ systems.

Type of symmetry	Relations among the coupling constants	No. of independent parameters	Subgroup of $H_{Z_2\otimes Z_2\otimes Z_2}$	Global symmetry	Order of the group	No. of isomorphic groups
a	---	8	1	$Z_2\otimes Z_2\otimes Z_2$	8	
b	$a_{100}=a_{011}; a_{010}=a_{101}$ $b_{100}=b_{010}; b_{001}=b_{111}$	6	Z_2	$Z_2\otimes(Z_2 \wr Z_2)$	16	21
c	$a_{100}=a_{010}=a_{101}=a_{011}$ $b_{100}=b_{010}; b_{001}=b_{111}; b_{101}=b_{011}$	5	$Z_2\otimes Z_2$	$Z_2 \wr (Z_2\otimes Z_2)$	64	7
d	$a_{100}=a_{011}; a_{010}=a_{101}; a_{001}=a_{110}$ $b_{100}=b_{010}=b_{001}=b_{111}$	5	$Z_2\otimes Z_2$	$(Z_2\otimes Z_2)\wr Z_2$	32	7
e	$a_{100}=a_{010}=a_{101}=a_{011}; a_{001}=a_{110}$ $b_{100}=b_{010}=b_{001}=b_{111}; b_{011}=b_{101}$	4	$Z_2\sim Z_2$	$Z_2 \wr Z_2 \wr Z_2$	128	21
f	$a_{100}=a_{010}=a_{001}; a_{110}=a_{011}=a_{101}$ $b_{100}=b_{010}=b_{001}; b_{110}=b_{011}=b_{101}$	4	S_3	$Z_2\otimes S_4$	48	28
g	$a_{100}=a_{010}=a_{101}=a_{011}; a_{110}=a_{001}=a_{111}$ $b_{100}=b_{010}=b_{001}=b_{011}=b_{101}=b_{111}$	3	S_4	$Z_2 \wr S_4$	384	7
h	$a_{100}=a_{010}=a_{001}=a_{110}=a_{101}=a_{011}$ $b_{100}=b_{010}=b_{001}=b_{111}; b_{110}=b_{101}=b_{011}$	3	S_4	$S_4 \wr Z_2$	1152	7
i	$a_{100}=a_{010}=a_{001}=a_{110}=a_{101}=a_{011}=a_{111}$ $b_{100}=b_{010}=b_{001}=b_{110}=b_{101}=b_{011}=b_{111}$	2	$H_{Z_2\otimes Z_2\otimes Z_2}$	S_8	40320	1

The Lagrangian function corresponding to a certain global symmetry G is best written in the orbit parametrization

$$L(\hat{\alpha}) = \sum_{i=1}^{t} b_{\theta_i} \sum_{\hat{\beta}_i \in \theta_i} \delta(\hat{\alpha} - \hat{\beta}_i). \tag{A3}$$

Here θ_i denote the various orbits corresponding to G (if G coincides with A each orbit has one element $\hat{\beta}$). By convention we take $L(0) = (0)$ and assume

$$b_{\theta_t} > b_{\theta_{t-1}} > \ldots > b_{\theta_1} > 0; \tag{A4}$$

this makes our system ferromagnetic.

The transfer matrix T is defined in the usual way:

$$\begin{aligned}\langle \hat{\alpha}_\mu^1, \ldots, \hat{\alpha}_\mu^M | T | \hat{\alpha}_{\mu+1}^1, \ldots, \hat{\alpha}_{\mu+1}^M \rangle &= \langle \hat{\alpha}_\mu | T | \hat{\alpha}_{\mu+1} \rangle \\ &= \exp\Big\{ -\xi_C \sum_{s=1}^{M} L(\hat{\alpha}_\mu^s - \hat{\alpha}_{\mu+1}^s) \\ &\quad - \xi_D \sum_{s=1}^{M} L(\hat{\alpha}_\mu^s - \hat{\alpha}_\mu^{s+1}) \Big\}\end{aligned} \tag{A5}$$

and we have

$$W = \mathrm{Tr}(T^M). \tag{A6}$$

We are interested in the limit $\xi_C \to \infty$, $\xi_D \to 0$ of the transfer matrix. In this limit due to our assumption (A4) the only non-negligible matrix elements of T are those corresponding to "no-flips" and those corresponding to the "flips" given by the orbit b_{θ_1}. We can now define our limit in a precise way by requiring the parameter

$$\lambda = \xi_D e^{\xi_C b_{\theta_1}} \tag{A7}$$

to remain fixed. We have

$$\begin{aligned}\langle \hat{\alpha}_\mu | T | \hat{\alpha}_{\mu+1} \rangle \approx{}& \delta(\hat{\alpha}_\mu - \hat{\alpha}_{\mu+1}) \\ &- \frac{\xi_D}{\lambda} \Big\{ \lambda \delta(\hat{\alpha}_\mu - \hat{\alpha}_{\mu+1}) \times \sum_{s=1}^{M} L(\hat{\alpha}_\mu^s - \hat{\alpha}_\mu^{s+1}) \\ &- \big[f(\hat{\alpha}_\mu^1 - \hat{\alpha}_{\mu+1}^1) \delta(\hat{\alpha}_\mu^2 - \hat{\alpha}_{\mu+1}^2) \cdots \delta(\hat{\alpha}_\mu^M - \hat{\alpha}_{\mu+1}^M) + \\ &+ \delta(\hat{\alpha}_\mu^1 - \hat{\alpha}_{\mu+1}^1) f(\hat{\alpha}_\mu^2 - \hat{\alpha}_{\mu+1}^2) \cdots \delta(\hat{\alpha}_\mu^M - \alpha_{\mu+1}^M) \\ &+ \cdots \\ &+ \delta(\hat{\alpha}_\mu^1 - \hat{\alpha}_{\mu+1}^1) \delta(\hat{\alpha}_\mu^2 - \hat{\alpha}_{\mu+1}^2) \cdot f(\hat{\alpha}_\mu^M - \hat{\alpha}_{\mu+1}^M) \big] \Big\}.\end{aligned} \tag{A8}$$

In Eq. (A8)

$$f(\hat{\alpha}) = \sum_{\hat{\beta}_i \in \theta_i} \delta(\hat{\alpha} - \hat{\beta}). \tag{A9}$$

We now write $L(\hat{\alpha})$ of Eq. (A8) in the character parametrization

$$L(\hat{\alpha}) = \sum_{\hat{r} \neq 0} \bar{a}_{\hat{r}} - \sum_{\hat{r} \neq 0} \bar{a}_{\hat{r}} \chi_{\hat{r}}(\hat{\alpha}) \tag{A10}$$

($\bar{a}_{\hat{r}} = -a_{\hat{r}}$) and get

$$T = 1 - \xi_D M \sum_{\hat{r} \neq 0} \bar{a}_{\hat{r}} - \frac{\xi_D}{\lambda} H, \tag{A11}$$

where H is the Hamiltonian of the system. Before writing it down it is useful to introduce some notations.

We define the matrices $\Gamma_{\hat{\beta}}(s)$ and $\sigma_{\hat{r}}(s)$:

$$\begin{aligned}&\langle \hat{\alpha}_\mu^1, \ldots, \hat{\alpha}_\mu^M | \Gamma_{\hat{\beta}}(s) | \hat{\alpha}_{\mu+1}^1, \ldots, \hat{\alpha}_{\mu+1}^M \rangle \\ &= \delta(\hat{\alpha}_\mu^1 - \hat{\alpha}_{\mu+1}^1) \cdots \delta(\hat{\alpha}_\mu^s - \hat{\alpha}_{\mu+1}^s - \hat{\beta}) \cdots \delta(\hat{\alpha}_\mu^M - \hat{\alpha}_{\mu+1}^M),\end{aligned} \tag{A12}$$

$$\begin{aligned}&\langle \hat{\alpha}_\mu^1, \ldots, \hat{\alpha}_\mu^M | \sigma_{\hat{r}}(s) | \hat{\alpha}_{\mu+1}^1, \ldots, \hat{\alpha}_{\mu+1}^M \rangle \\ &= \delta(\hat{\alpha}_\mu^1 - \hat{\alpha}_{\mu+1}^1) \cdots \delta(\hat{\alpha}_\mu^M - \hat{\alpha}_{\mu+1}^M) \chi_{\hat{r}}(\hat{\alpha}_\mu^s).\end{aligned} \tag{A13}$$

In these notations the Hamiltonian reads

$$H = -\lambda \sum_{s=1}^{M} \sum_{\hat{r} \neq 0} \bar{a}_{\hat{r}} \sigma_{\hat{r}}(s) \sigma_{-\hat{r}}(s+1) - \sum_{s=1}^{M} \sum_{\hat{\beta}_i \in \theta_i} \Gamma_{\hat{\beta}_i}(s). \tag{A14}$$

It is crucial to observe that the "spin-flip" matrices $\Gamma_{\hat{\beta}_i}(s)$ which appear in Eq. (A14) are those given by the orbit structure of the Lagrangian which in turn is given by both the global symmetry and dynamics [see Eq. (A4)].

Hamiltonians of the type (A14) might be self-dual in the sense that the spectrum verifies the condition[8]

$$E(\lambda) = \lambda E(1/\lambda). \tag{A15}$$

Leaving aside the very delicate problem of the boundary conditions, and repeating the same arguments as for Potts models,[1] one can show that the system is self-dual if

$$\sum_{\hat{r} \neq 0} \bar{a}_{\hat{r}} \delta(\hat{\alpha} - \hat{r}) = \sum_{\hat{\beta}_1 \in \theta_t} \delta(\hat{\alpha} - \hat{\beta}_1). \tag{A16}$$

We now consider two examples:

(a) A Z_3 system

We consider a spin system having only Z_3 as a global symmetry given by the Lagrangian

$$L(\alpha_P - \alpha_{P'}) = 2\cos\left(\frac{2\pi}{3}\epsilon\right) - 2\cos\frac{2\pi}{3}(\epsilon + \alpha_P - \alpha_{P'}), \quad \alpha_P, \alpha_{P'} \in Z_3 \tag{A17}$$

where ϵ is a parameter ($\epsilon < \frac{1}{2}$). This interaction is not symmetric!

$$L(\alpha_P - \alpha_{P'}) \neq L(\alpha_{P'} - \alpha_P). \tag{A18}$$

We have

$$L(\alpha) = b_1 \delta(\alpha - 1) + b_2 \delta(\alpha - 2) \tag{A19}$$

with

$$b_1 > b_2 > 0. \tag{A20}$$

From (A17) we derive

$$\bar{a}_1 = \frac{e^{(2\pi i/3)\epsilon}}{2}, \quad \bar{a}_2 = \bar{a}_1^* \tag{A21}$$

and the Hamiltonian reads

$$\begin{aligned}H = -\lambda \sum_{s=1}^{M} &(e^{(2\pi i/3)\epsilon} \sigma_1(s) \sigma_1^+(s+1) + e^{(-2\pi i/3)\epsilon} \sigma_1^+(s) \sigma_1(s+1)) \\ &- \sum_{s=1}^{M} \Gamma_2(s),\end{aligned} \tag{A22}$$

where

$$\sigma_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & e^{2\pi i/3} & 0 \\ 0 & 0 & e^{-2\pi i/3} \end{pmatrix}, \quad \Gamma_2 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \tag{A23}$$

The Hamiltonian (A22) is obviously not hermitian, but the system might still have interesting properties.

(b) A Z_{13} system with M_{13}^6 global symmetry

We consider the Lagrangian

$$L(\alpha) = 6 - 2\left(\cos\frac{2\pi\alpha}{13} + \cos\frac{6\pi\alpha}{13} + \cos\frac{8\pi\alpha}{13}\right), \quad \alpha \in Z_{13}. \tag{A24}$$

One has

$$\bar{a}_1 = \bar{a}_3 = \bar{a}_4 = \bar{a}_9 = \bar{a}_{10} = \bar{a}_{12} = 1,$$
$$\bar{a}_2 = \bar{a}_5 = \bar{a}_6 = \bar{a}_7 = \bar{a}_8 = \bar{a}_{11} = 0 \tag{A25}$$

and

$$L(\alpha) = b_{\theta_1}(\delta(\alpha-1)+\delta(\alpha-3)+\delta(\alpha-4)+\delta(\alpha-9) + \delta(\alpha-10)+\delta(\alpha-12)) + b_{\theta_2}(\delta(\alpha-2) + \delta(\alpha-5)+\delta(\alpha-6)+\delta(\alpha-7)+\delta(\alpha-8) + \delta(\alpha-11)), \tag{A26}$$

with

$$b_{\theta_1} > b_{\theta_2} > 0. \tag{A27}$$

One can check that the relation (A16) is satisfied and the Hamiltonian is self-dual.

Other Hamiltonians with the Same Global Symmetry as A Systems

Quantum systems described by Eq. (A14) are a special case of a more general class of systems:

$$H = T + V, \tag{A28}$$

where the kinetic energy T and the potential energy V have the form

$$T = \sum_{s=1}^{M} \sum_{\hat{r}\neq 0} A_{\hat{r}} \sigma_{\hat{r}}(s)\sigma_{-\hat{r}}(s+1), \tag{A29}$$

$$V = \sum_{s=1}^{M} \sum_{\hat{\beta}\neq 0} B_{\hat{\beta}} \Gamma_{\hat{\beta}}(s). \tag{A30}$$

Here $A_{\hat{r}}$ and $B_{\hat{\beta}}$ are arbitrary coupling constants (notice that we have $2|A| - 2$ free parameters). The Hamiltonian (A28) has the abelian group A as global symmetry. Higher global symmetries are obtained if the parameters $A_{\hat{r}}$ and $B_{\hat{\beta}}$ verify the same relations as the parameters $a_{\hat{r}}$ and $b_{\hat{\beta}}$ of the Lagrangian (see, for example, Table I).

Quantum systems described by (A28)–(A30) are of interest on their own and some of them could be completely integrable. It was already shown[19] that at the critical point, Z_n systems with S_n global symmetry have an infinite set of conservation laws. In the Z_2 case the solution is known analytically.[20] As an example we consider a quantum system given by the Hamiltonian

$$H = A_1 \sum_s \sigma_1(s)\sigma_1^+(s+1) + A_2 \sum_s \sigma_1^+(s)\sigma_1(s+1) + B_1 \sum_s \Gamma_1(s) + B_2 \sum_s \Gamma_2(s), \tag{A31}$$

where

$$\Gamma_1(s) = \Gamma_2^+(s) \tag{A32}$$

and $\sigma_1(s)$, $\Gamma_2(s)$ are given by Eq. (A23). If we choose

$$A_2 = A_1^*, \quad B_2 = B_2^* \tag{A33}$$

the Hamiltonian (A31) is Hermitian and has only Z_3 symmetry. This is a very interesting system which, to our knowledge, has not yet been studied.

APPENDIX B: THE FACTORIZATION OF THE PARTITION FUNCTION

Let us consider an $\bar{A}$ system where the $\bar{A}$ group is the direct product of two abelian groups A_1 and A_2

$$\bar{A} = A_1 \otimes A_2. \tag{B1}$$

If the Lagrangian function has the special form

$$L(\bar{\alpha}) = L_1(\alpha_1) + L_2(\alpha_2)$$
$$(\bar{\alpha}\in\bar{A}, \quad \alpha_1\in A_1, \quad \alpha_2\in A_2), \tag{B2}$$

The partition function factorizes into the product of two partition functions, one with the Lagrangian $L_1(\alpha_1)$ and the other with $L_2(\alpha_2)$. The global symmetry of the $\bar{A}$ system given by Eq. (B2) is

$$G_1 \otimes G_2, \tag{B3}$$

where $G_1(G_2)$ is the global symmetry of $L_1(L_2)$. If $A_1 = A_2$ and $L_1(\alpha_1) = L_2(\alpha_2)$ the global symmetry is

$$G_1 \wr Z_2 = G_2 \wr Z_2. \tag{B4}$$

This observation looks trivial but is has important implications:

(1) If $L(\bar{\alpha})$ has one of the symmetries (B3) or (B4) one knows that for special values of the coupling constants one has factorization. This does not occur only if the Lagrangian has the "diagonalized" form (B2) but can happen also if $L(\bar{\alpha})$ is obtained from (B2) through a change of basis given by an element of the automorphism group.

(2) Consider an A system which cannot be written in the form (B1) but we have $|A| = |\bar{A}|$ (take, for example, $A = Z_9$ and $\bar{A} = Z_3 \otimes Z_3$). If the global symmetry G of the A system is of the type (B3) or (B4) one knows that for special choices of the coupling constants of the A system one has factorization. The corresponding coupling constants can be obtained mapping the A system into the $\bar{A}$ system.

As an example we consider the well-known case of the $Z_2 \otimes Z_2$ system[9,13] (see also Sec. 5).

We first notice that the following $Z_2 \otimes Z_2$ systems factorize into two independent Ising systems:

(a) $Z_2 \otimes Z_2$ *global symmetry*

$$a_{1,0}(-1)^{\alpha_1} + a_{0,1}(-1)^{\alpha_2}, \quad (\alpha_1,\alpha_2\in Z_2). \tag{B5}$$

$$a_{1,0}(-1)^{\alpha_1} + a_{1,1}(-1)^{\alpha_1+\alpha_2},$$

(b) $Z_2 \wr Z_2$ *global symmetry*

$$a_{1,0}[(-1)^{\alpha_1} + (-1)^{\alpha_2}], \tag{B6a}$$

$$a_{1,0}[(-1)^{\alpha_1} + (-1)^{\alpha_1+\alpha_2}]. \tag{B6b}$$

Consider now a Z_4 system with a $Z_2 \wr Z_2$ global symmetry:

$$L(\alpha) = 2a_1 \cos(\pi\alpha/2) + a_2(-1)^{\alpha}, \quad \alpha\in Z_4. \tag{B7}$$

This system can be mapped into a $Z_2 \otimes Z_2$ system with the same global symmetry [see Eqs. (5.4)]. The mapping is

$$0\to(0,0), \quad 1\to(0,1), \quad 2\to(1,1), \quad 3\to(1,0). \tag{B8}$$

If we take $a_2 = 0$, (B7) is mapped into (B6a) and one has factorization. We have thus recovered the known fact that the vector Potts Z_4 model factorizes.

Our considerations can be extended in a trivial way to the case in which $\bar{A}$ in Eq. (B1) is the direct product of more than two groups.

APPENDIX C: SOME COMMENTS ON SPIN SYSTEMS DEFINED ON NONABELIAN MANIFOLDS

A spin system can be defined not only on abelian manifolds but also on nonabelian groups. Consider a nonabelian group B with group elements g. The Lagrangian function is

$$L(g_P, g_{P'}) = L(g_P g_{P'}^{-1}) g_P, g_{P'} \in B. \tag{C1}$$

This expression coincides with Eq. (1.10) in the abelian case. The analoges of Eqs. (1.13) and (1.14) are

$$L(g) = \sum_{r,m,n} a^{\lambda}_{m,n} T^{\lambda}_{m,n}(g) \tag{C2}$$

and

$$L(g) = \sum_{g' \in B} b_{g'} \delta(g, g'). \tag{C3}$$

In Eq. (C2) $T^{\lambda}_{m,n}(g)$ are the matrix elements of the irreducible representation λ of B. The function $\delta(g,g')$ in Eq. (C3) is equal to one if g coincides with g' and zero otherwise.

The Lagrangian function (C1) has obviously B itself as a global symmetry but (like in the abelian case) for special choices of the coupling constants $a^{\lambda}_{m,n}$ or b_g, the global symmetry may be larger.

A spin system defined on B can be rewritten as a spin system defined on an abelian group A ($|A| = |B|$) if for a given global symmetry G of $L(g)$ there exists an A system with the same global symmetry G. This is possible if G contains A as a regular subgroup.

As a trivial example consider a B system with the interaction

$$L(g) = b_e \delta(g,e), \tag{C4}$$

where e is the unit element of B. This system has obviously $S_{|B|}$ as a global symmetry and is identical to the $|B|$-component Potts model given by Eq. (1.18), which is defined on $Z_{|B|}$.

Writing a B system as an A system is important because for A systems one has the duality transformation.

Several authors[12] have considered spin systems having a manifold B which is a semidirect product of abelian groups:

$$B = ((A_1, \circledS A_2) \circledS \cdots) \circledS A_n \tag{C5}$$

and a Lagrangian which is a *class function of* B (this corresponds to taking $a^{\lambda}_{m,n} = \delta_{m,n} a_{\lambda}$ in Eq. (C2). These authors have shown that one can rewrite the B system as an A system with

$$A = A_1 \otimes A_2 \otimes \cdots \otimes A_n \tag{C6}$$

(The rewriting procedure has a simple group theoretical significance which will be discussed in detail in paper III). This observation led to the erroneous opinion that the only B systems which admit a duality transformation are systems where the *global symmetry* is of the type (C5).

By now we are in a position to settle this point. First of all as stated before [see example (C4)] the manifold B does not have to be of the form (C5) in order to write it as an A system. Secondly, the global symmetry G is at least as large as to contain B [Eq. (C5)] *and* A [Eq. (C6)] as subgroups. In fact we show in Paper III that G is at least $(B \otimes B)/C$, where C is the center of B.

As an example consider the nonabelian group D_4 of order 8. It is easy to show that if the Lagrangian is a class function on D_4, the D_4 system can be mapped in a $Z_2 \otimes Z_2 \otimes Z_2$ system with the Lagrangian:

$$\begin{aligned} L(\hat{\alpha}) = a_{0,0,0} + a_{1,0,0}[(-1)^{\alpha_1} + (-1)^{\alpha_2} + (-1)^{\alpha_1+\alpha_2} \\ + (-1)^{\alpha_2+\alpha_3}] + a_{0,0,1}(-1)^{\alpha_3} + a_{1,1,0}(-1)^{\alpha_1+\alpha_2} \\ + a_{1,1,1}(-1)^{\alpha_1+\alpha_2+\alpha_3}. \end{aligned} \tag{C7}$$

The global symmetry of this system is known (see Table I): it is $Z_2 \wr (Z_2 \otimes Z_2)$, which is a group os order 64 and which indeed contains $Z_2 \otimes Z_2 \otimes Z_2$ and $D_4 \simeq Z_2 \wr Z_2$ as subgroups.

APPENDIX D: THE AUTOMORPHISM GROUP OF $Z_2 \otimes Z_2 \otimes Z_2$

The group $H_{Z_2 \otimes Z_2 \otimes Z_2}$ of order 168 has a representation given by 3×3 matrices with entries in Z_2 (see Sec. 3). Its group elements are given by 28 cycles of order 3, 21 cycles of order 4, and 8 cycles of order 7. We give here an element of each cycle. The matrices denoted by A, B, and C are used in Sec. 5.

Cycles of Order Three

$$A = \begin{pmatrix}010\\001\\100\end{pmatrix}\begin{pmatrix}110\\100\\101\end{pmatrix}\begin{pmatrix}001\\011\\101\end{pmatrix}\begin{pmatrix}110\\011\\010\end{pmatrix}\begin{pmatrix}101\\010\\110\end{pmatrix}\begin{pmatrix}100\\011\\100\end{pmatrix}$$
$$\begin{pmatrix}011\\010\\101\end{pmatrix}\begin{pmatrix}100\\111\\110\end{pmatrix}\begin{pmatrix}110\\101\\001\end{pmatrix}\begin{pmatrix}111\\100\\001\end{pmatrix}\begin{pmatrix}111\\001\\011\end{pmatrix}\begin{pmatrix}001\\111\\101\end{pmatrix}$$
$$\begin{pmatrix}010\\110\\101\end{pmatrix}\begin{pmatrix}111\\011\\010\end{pmatrix}\begin{pmatrix}101\\111\\100\end{pmatrix}\begin{pmatrix}010\\110\\111\end{pmatrix}\begin{pmatrix}010\\110\\001\end{pmatrix}\begin{pmatrix}100\\011\\010\end{pmatrix}$$
$$\begin{pmatrix}101\\010\\100\end{pmatrix}\begin{pmatrix}111\\010\\100\end{pmatrix}\begin{pmatrix}100\\001\\111\end{pmatrix}\begin{pmatrix}011\\110\\001\end{pmatrix}\begin{pmatrix}010\\011\\111\end{pmatrix}\begin{pmatrix}010\\101\\110\end{pmatrix}$$
$$\begin{pmatrix}111\\110\\010\end{pmatrix}\begin{pmatrix}011\\101\\100\end{pmatrix}\begin{pmatrix}111\\001\\101\end{pmatrix}\begin{pmatrix}110\\111\\100\end{pmatrix}.$$

Cycles of Order Four

$$B = \begin{pmatrix}001\\100\\111\end{pmatrix}\begin{pmatrix}010\\001\\111\end{pmatrix}\begin{pmatrix}001\\111\\010\end{pmatrix}\begin{pmatrix}011\\101\\111\end{pmatrix}\begin{pmatrix}011\\111\\110\end{pmatrix}\begin{pmatrix}111\\101\\110\end{pmatrix}$$
$$\begin{pmatrix}100\\101\\010\end{pmatrix}\begin{pmatrix}011\\010\\100\end{pmatrix}\begin{pmatrix}011\\100\\001\end{pmatrix}\begin{pmatrix}111\\010\\011\end{pmatrix}\begin{pmatrix}100\\111\\101\end{pmatrix}\begin{pmatrix}110\\011\\001\end{pmatrix}\begin{pmatrix}100\\110\\111\end{pmatrix}$$
$$\begin{pmatrix}110\\010\\101\end{pmatrix}\begin{pmatrix}101\\111\\001\end{pmatrix}\begin{pmatrix}001\\110\\100\end{pmatrix}\begin{pmatrix}110\\001\\010\end{pmatrix}\begin{pmatrix}010\\100\\011\end{pmatrix}\begin{pmatrix}101\\100\\110\end{pmatrix}\begin{pmatrix}011\\110\\010\end{pmatrix}\begin{pmatrix}110\\101\\100\end{pmatrix}.$$

Cycles of Order Seven

$$C = \begin{pmatrix}110\\101\\010\end{pmatrix}\begin{pmatrix}101\\001\\110\end{pmatrix}\begin{pmatrix}001\\101\\010\end{pmatrix}\begin{pmatrix}110\\101\\111\end{pmatrix}\begin{pmatrix}011\\001\\111\end{pmatrix}$$
$$\begin{pmatrix}011\\111\\101\end{pmatrix}\begin{pmatrix}111\\110\\011\end{pmatrix}\begin{pmatrix}001\\100\\110\end{pmatrix}.$$

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The global symmetries of spin systems defined on abelian groups. II

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(Received 10 February 1981; accepted for publication 18 May 1981)

We present the classification of the global symmetry groups of spin systems defined on $Z_p \otimes Z_q$, Z_{p^2}, and $Z_p \otimes Z_p$ abelian groups (p and q are prime numbers).

PACS numbers: 02.20.Km

1. INTRODUCTION

In the previous paper[1] (to be referred to as I) we have shown under which circumstances an abelian spin system has a global symmetry larger than the abelian group on which the system has been defined. We have given the classification of the global symmetries of systems defined on Z_p (p prime), $Z_2 \otimes Z_2$, and $Z_2 \otimes Z_2 \otimes Z_2$. We have also discussed several physical consequences.

We assume that by now the reader is familiar with the definition of a global symmetry G [Eq. I(1.20)], with the symmetry $\tilde{G}$ of the dual system [Eq. I(1.25)], with automorphisms and affine groups (I, Sec. 2) and with wreath products (I, Sec. 4). We also hope that the detailed presentation of the $Z_2 \otimes Z_2 \otimes Z_2$ case has made clear how to use G in order to find symmetry relations for the generating functional [see Eqs. I (5.2) and (5.3)].

In the present paper we give a complete classification of the global symmetries for spin systems defined on $Z_p \otimes Z_q$ (Sec. 2), Z_{p^2} (Sec. 3), and $Z_p \otimes Z_p$ (Sec. 4). Here p and q are prime numbers. The proofs will be given elsewhere.[2] The simple cases $Z_2 \otimes Z_3$, Z_9, and $Z_3 \otimes Z_3$ are given as applications in Tables I–IV. (The Z_4 case is trivial and the $Z_2 \otimes Z_2$ case was already considered in Ref. 1.)

Before we start the presentation of our results we would like to introduce two definitions. The Lagrangian density

$$L = L(\hat{\alpha}_p - \hat{\alpha}_{p'}), \quad \hat{\alpha}_p, \hat{\alpha}_{p'} \in A \tag{1.1}$$

has the global symmetry G if

$$L(g(\hat{\alpha}_p) - g(\hat{\alpha}_{p'})) = L(\hat{\alpha}_p - \hat{\alpha}_{p'}), \quad g \in G. \tag{1.2}$$

It can be shown that the transformation g can be written in the form

$$\hat{\alpha}' = g(\hat{\alpha}) = (g_0, \hat{t})(\hat{\alpha}) = g_0(\hat{\alpha}) + \hat{t}, \tag{1.3}$$

where $\hat{t} \in A$ and $g_0 \in G_0$. G_0 is the subgroup of G which leaves the origin $\hat{\alpha} = 0$ unchanged (*the little group of the origin*). The automorphisms U [see Eq. I(2.1)] form a subgroup of G_0. From Eq. (1.3) it is clear that G_0 determines uniquely G. We now show how G_0 determines L.

We look at L as a function of a single variable,

$$L = L(\hat{\alpha}), \quad \hat{\alpha} \in A. \tag{1.4}$$

Equation (1.2) implies

$$L(g_0(\hat{\alpha})) = L(\hat{\alpha}), \quad g_0 \in G_0. \tag{1.5}$$

A set of elements $\hat{\alpha}_1^{(1)}, \hat{\alpha}_2^{(1)}, \ldots, \hat{\alpha}_s^{(1)} \in A$ form an *orbit* θ_1 *of* G_0 *on* A if

$$\hat{\alpha}_i^{(1)} = g_0(\hat{\alpha}_1^{(1)}), \quad i = 2, \ldots, s, \; g_0 \in G. \tag{1.6}$$

Obviously A is a reunion of disjunct orbits of G_0. The Lagrange density L has by Eq. (1.5) the same value on an orbit and thus L is completely specified by giving the orbits of G_0 on A. In the "orbit" parametrization of the Lagrangian [see Eq. I (1.14)],

$$L(\hat{\alpha}) = \sum_{\hat{\beta} \in A} b_{\hat{\beta}} \delta(\hat{\alpha} - \hat{\beta}). \tag{1.7}$$

The coefficients $b_{\hat{\beta}}$ are the same for all $\hat{\beta}$'s belonging to the same orbit of G_0.

We now proceed to present our classification.

2. $Z_p \otimes Z_q$ SYSTEMS (p AND q ARE PRIMES)

An element of $Z_p \otimes Z_q$ is a double (α_1, α_2) with $\alpha_1 = 0,1,\ldots,p-1; \alpha_2 = 0,1,\ldots,q-1$. The group law is addition modulo p for the first component and addition modulo q for the second one:

$$(\alpha_1, \alpha_2) + (\alpha_1', \alpha_2') = (\alpha_1 + \alpha_1', \alpha_2 + \alpha_2'). \tag{2.1}$$

The group of automorphisms of $Z_p \otimes Z_q$ (denoted by $H_{Z_p \otimes Z_q}$) is the direct product of the group of automorphisms of Z_p with that of Z_q (see I, Sec. 2). Thus an automorphism is a double (u_1, u_2) with $u_1 = 1,\ldots,p-1; u_2 = 1,\ldots,q-1$ and it has the following action on $Z_p \otimes Z_q$:

$$(u_1, u_2)(\alpha_1, \alpha_2) = (u_1\alpha_1, u_2\alpha_2). \tag{2.2}$$

The group law in $H_{Z_p \otimes Z_q}$ is

$$(u_1, u_2)(u_1', u_2') = (u_1u_1', u_2u_2'). \tag{2.3}$$

In Eqs. (2.2) and (2.3) the multiplications are modulo p for the first component and modulo q for the second one.

The group $Z_p \otimes Z_q$ is isomorphic to the group Z_{pq}, i.e., to the additive group of integers modulo pq. The mapping between the two is

$$(\alpha_1, \alpha_2) \in Z_p \otimes Z_q \leftrightarrow \alpha_1 q + \alpha_2 p \in Z_{pq}. \tag{2.4}$$

An automorphism of Z_{pq} is a multiplication (modulo pq) by an integer u which is not divisible by either p or q. Thus there are $(p-1)(q-1)$ automorphisms. The mapping between $H_{Z_p \otimes Z_q}$ and $H_{Z_{pq}}$ is

$$H_{Z_p \otimes Z_q} \ni (u_1, u_2) \leftrightarrow u = \left[\frac{u_1}{q} (\mathrm{mod} p)\right] q + \left[\frac{u_2}{p} (\mathrm{mod} q)\right] p. \tag{2.5}$$

Equations (2.2) and (2.3) become

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$$u(\alpha_1 q + \alpha_2 p) = u_1\alpha_1 q + u_2\alpha_2 p \pmod{pq}, \tag{2.6}$$

$$uu' = \left[\frac{u_1u_1'}{q} \pmod{p}\right]q + \left[\frac{u_2u_2'}{p} \pmod{q}\right]p \pmod{pq}. \tag{2.6'}$$

We now give a complete list of the possible global symmetries of $Z_p \otimes Z_p$ systems. The proof that there are no other possibilities will be given in Ref. 2.

There are three classes of global symmetries.

Class 1: *The orbits of* G_0 *on* $Z_p \otimes Z_q$ *are completely determined by a subgroup of* $H_{Z_p \otimes Z_q}$.

In order to give an explicit result we have to specify the subgroups of $H_{Z_p \otimes Z_q}$. First we note that $H_{Z_p}(H_{Z_q})$ is cyclic of order $p-1(q-1)$. If $v(w)$ is a generator of $H_{Z_p}(H_{Z_q})$, then every automorphism of $Z_p \otimes Z_q$ has the form

$$u = (v^i, w^j) \tag{2.7}$$

with $i = 1,...,p-1$ and $j = 1,...,q-1$. Note that

$$v^{p-1} = 1 \pmod{p}, \quad w^{q-1} = 1 \pmod{q} \tag{2.8}$$

but

$$v^i \neq 1 \pmod{p}, \quad w^j \neq 1 \pmod{q}, \quad i < p-1, j < q-1. \tag{2.8'}$$

A subgroup of $H_{Z_p \otimes Z_q}$ is characterized by three integers m, n, and s such that

$$\begin{aligned} &ms \text{ divides } p-1, \\ &ns \text{ divides } q-1. \end{aligned} \tag{2.9}$$

It consists of the following automorphisms:

$$(v^{[(p-1)/ms](is+r)}, w^{[(q-1)/ms](js+r)}); \quad i = 1,...,m; j = 1,...,n; r = 1,...,s. \tag{2.10}$$

We denote this subgroup by $H_{m,n;s}$. The group obtained by combining the automorphisms from $H_{m,n;s}$ with $Z_p \otimes Z_q$ translations will be denoted by $M_{p,q}^{m,n;s}$. It is the semidirect product of $Z_p \otimes Z_q$ with $H_{m,n;s}$. Note that

$$M_{p,q}^{m,n;1} = M_p^m \otimes M_q^n \tag{2.11}$$

(the groups M_p^m and M_q^n have been defined in Ref. 1).

We now sum up our results on symmetries of Class 1: To every subgroup $H_{m,n;s}$ of $H_{Z_p \otimes Z_q}$ there corresponds a global symmetry of the $Z_p \otimes Z_q$ system. The Lagrangian density is given by the orbits of $H_{m,n;s}$ on $Z_p \otimes Z_q$. The orbits are determined using Eqs. (2.2) and (2.10). The corresponding maximal symmetry grouup is $G = M_{p,q}^{m,n;s}$ except for the following cases:

(a) $s = 1, m = p-1; n \neq q-1$ when $G = S_p \otimes M_q^n$;

(b) $s = 1; m \neq p-1; n = q-1$ when $G = M_p^m \otimes S_q$;

(c) $s = 1, m = p-1, n = q-1$ when $G = S_p \otimes S_q$.

Class 2: *G is a wreath product.*

Let us write $Z_p \otimes Z_q$ in the following form:

$$\begin{aligned} &(0,0),(0,1),...,(0,q-1), \\ &(1,0),(1,1),...,(1,q-1), \\ &\quad\cdot\quad\cdot\quad\cdot\quad\cdot \\ &(p-1,0),(p-1,1),...,(p-1,q-1). \end{aligned} \tag{2.12}$$

The first row is the subgroup Z_q and the first column the subgroup Z_p.

A general permutation from S_{pq} acts on the elements of this tableau at random, preserving neither the row nor the column structure.

Let us now consider permutations that map each column of (2.12) into another column. In Sec. 4 of Paper I we learned that the set of all such permutations forms the group $S_p \sim S_q$. Similarly the set of all permutations that map each row of (2.12) into another row forms the group $S_q \sim S_p$. The permutations which have both properties form the group $S_p \otimes S_q$. Therefore each symmetry group of Class 1 preserves both the row and the column structure of (2.12).

We say that a symmetry group is of Class 2 if it is a subgroup of $S_p \sim S_q$ or of $S_q \sim S_p$, but not a subgroup of $S_p \otimes S_q$. We proved the following result: The symmetry groups of Class 2 are $M_p^m \sim M_q^n$ and $M_q^n \sim M_p^m$. If $m = p-1$ or (and) $n = q-1$ the corresponding maximal symmetry group is obtained by replacing M_p^m with S_p or (and) M_q^n with S_q. Note the form of the Lagrangian density: if $G = M_p^m \sim M_q^n$, then

$$L(\alpha_1,\alpha_2) = L_1(\alpha_1)\delta(\alpha_2) + L_2(\alpha_2), \tag{2.13}$$

where $L_1(L_2)$ corresponds to a $Z_p(Z_q)$ system with global symmetry $M_p^m(M_q^n)$.

Class 3: *G does not preserve the row or the column structure of* (2.12).

A trivial consequence of a theorem by Schur (see Refs. 2 and 3) is: *The only symmetry group of Class* 3 *is* $G = S_{pq}$ and

$$L(\alpha_1,\alpha_2) = \delta(\alpha_1)\delta(\alpha_2), \quad \alpha_1 \in Z_p, \alpha_2 \in Z_q. \tag{2.14}$$

As an example consider the case $p = 2, q = 3$. In Table I we give a list of all maximal symmetry groups and the corresponding Lagrangians. (The notations are those of Ref. 1.)

We end this section with a comment concerning the connection between G and $\tilde{G}$. If G is of Class 1 or 3, then $G = \tilde{G}$. If $G = M_p^m \sim M_q^n$, then $\tilde{G} = M_q^n \sim M_p^m$.

TABLE I. The global symmetries of $Z_2 \otimes Z_3$ systems.

Global symmetry	Order of the group	Relations among the coupling constants
$Z_2 \otimes Z_3$	6	...
$Z_2 \otimes S_3$	12	$a_{0,1} = a_{0,2}, a_{1,1} = a_{1,2}$ $b_{0,1} = b_{0,2}, b_{1,1} = b_{1,2}$
$Z_3 \sim Z_2$	18	$a_{0,1} = a_{1,1}, a_{0,2} = a_{1,2}$ $b_{1,0} = b_{1,1} = b_{1,2}$
$Z_2 \sim Z_3$	24	$a_{1,0} = a_{1,1} = a_{1,2}$ $b_{0,1} = b_{1,1}, b_{0,2} = b_{1,2}$
$Z_2 \sim S_3$	48	$a_{0,1} = a_{0,2}, a_{1,0} = a_{1,1} = a_{1,2}$ $b_{0,1} = b_{0,2} = b_{1,1} = b_{1,2}$
$S_3 \sim Z_2$	72	$a_{0,1} = a_{0,2} = a_{1,1} = a_{1,2}$ $b_{0,1} = b_{0,2}, b_{1,0} = b_{1,1} = b_{1,2}$
S_6	720	$a_{1,0} = a_{0,1} = a_{0,2} = a_{1,1} = a_{1,2}$ $b_{1,0} = b_{0,1} = b_{0,2} = b_{1,1} = b_{1,2}$

3. Z_{p^2} SYSTEMS (p PRIME)

An element of Z_{p^2} is an integer $\alpha = 0,1,...p^2 - 1$. The group law is addition modulo p^2.

An automorphism of Z_{p^2} is a multiplication (modulo p^2) by an integer u which is not divisible by p:

$$u(\alpha) = u\alpha, \quad u \in H_{Z_{p^2}}, \alpha \in Z_{p^2}. \tag{3.1}$$

The group law in $H_{Z_{p^2}}$ is multiplication modulo p^2. $H_{Z_{p^2}}$ is cyclic of order $p(p-1)$. Let v be a generator of $H_{Z_{p^2}}$, i.e.,

$$v^{p(p-1)} = 1 \ (\mathrm{mod} p^2),$$
$$i = 1,2,...,p(p-1) - 1. \tag{3.2}$$
$$v^i \neq 1 \ (\mathrm{mod} p^2),$$

Denote by H_k the subgroup of order k [k divides $p(p-1)$] of $H_{Z_{p^2}}$ and by $M^k_{p^2}$ the group obtained by combining H_k with Z_{p^2} translations ($M^k_{p^2}$ is a metacyclic group[4]).

Similar to the Z_{pq} case, we divide the global symmetries G of Z_{p^2} into *three classes.* The proof that there are no other possibilities will be given in Ref. 2.
will be given in Ref. 2.

Class 1: $G = M^k_{p^2}$ *and* k *divides* $p - 1$.

The generator of H_k will be a power of v [see Eq. (3.2)]. The orbits of H_k on Z_{p^2} are determined using Eq. (3.1). $M^k_{p^2}$ is a maximal symmetry group.

Class 2: *G is a wreath product.*

Let us write the group Z_{p^2} as a square tableau, similar to Eq. (2.12):

$$\begin{array}{l} 0,p,2p,...,(p-1)p, \\ 1,p+1,2p+1,...,(p-1)p+1, \\ \quad . \quad . \quad . \quad . \quad . \\ p-1,p+(p-1),2p+(p-1),...,(p-1)p+(p-1). \end{array} \tag{3.3}$$

The first row is the subgroup Z_p. Each row is a coset from Z_{p^2}/Z_p (note that Z_{p^2}/Z_p is isomorphic to Z_p).

Every symmetry group of Class 2 will permute the rows amongst themselves. The role of the rows and columns cannot be interchanged as in the Z_{pq} case. This is a consequence of the fact that Z_{p^2} has only one subgroup. Thus every G of Class 2 will be a subgroup of $S_p \sim S_p$ with the first S_p acting on each row independently and the second S_p permuting the rows (see Sec. 4 of Paper I).

We proved the following result: The symmetry groups of Class 2 are $M^m_p \sim M^n_p$; whenever $m = p - 1$ or (and) $n = p - 1$, the corresponding maximal symmetry group is obtained by replacing M^m_p with S_p or (and) M^n_q with S_q.

Note that for $M^m_p \sim M^m_p$ the orbits are generated by the subgroup H_{pm} of $H_{Z_{p^2}}$. Note also that the symmetry groups of Class 1 preserve the row structure of Eq. (3.3) too.

Class 3: *G does not preserve the row structure of Eq.* (3.3).

Similiarly to the Z_{pq} case, *the only symmetry group of Class* 3 *is* $G = S_{p^2}$.

As an example consider the case $p = 3$. In Table II we give a list of all maximal symmetry groups and the corresponding orbits of G_0 on Z_9.

If G is of Class 1 or 3, then $G = \tilde{G}$. If $G = M^m_p \sim M^n_p$, then $\tilde{G} = M^n_p \sim M^m_p$.

TABLE II. The global symmetries of Z_9 systems.

Global symmetry	Order of the group	Relations among the coupling constants
Z_9	9	...
M^2_9	18	$b_1 = b_8, b_2 = b_7, b_3 = b_6, b_4 = b_5$
$Z_3 \sim Z_3$	81	$b_1 = b_4 = b_7, b_2 = b_5 = b_8$
$Z_3 \sim S_3$	162	$b_1 = b_2 = b_4 = b_5 = b_7 = b_8$
$S_3 \sim Z_3$	648	$b_3 = b_6, b_1 = b_4 = b_7, b_2 = b_5 = b_8$
$S_3 \sim S_3$	1296	$b_3 = b_6, b_1 = b_2 = b_4 = b_5 = b_7 = b_8$
S_9	9!	$b_1 = b_2 = b_3 = b_4 = b_5 = b_6 = b_7 = b_8$

4. $Z_p \otimes Z_p$ SYSTEMS

We have seen that the integer numbers close under two operations modulo p: addition and multiplication. The set of integers $0,1,...,p-1$ endowed with these two operations forms a field. We denote it by GF(p). This notation comes from the fact that finite fields are usually called Galois fields.[5] The distinction in notation between Z_p and GF(p) is not just academic. It will enable us to formulate the results more clearly.

An element of $Z_p \otimes Z_p$ is the double (α_1,α_2) with $\alpha_1,\alpha_2 \in \mathrm{GF}(p)$. Thus $Z_p \otimes Z_p$ is *a two-dimensional vector space over* GF(p). Its automorphisms are the basis transformations, i.e., the invertible matrices

$$U = \begin{pmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{pmatrix}, \quad u_{i,j} \in \mathrm{GF}(p); u_{11}u_{22} - u_{12}u_{21} \neq 0. \tag{4.1}$$

The group formed by all matrices (4.1) is denoted GL(2, p) (general linear group). It has the order $(p^2-1)(p^2-p)$. The group obtained by combining the $Z_p \otimes Z_p$ translations with GL(2, p) is denoted Aff(2, p) (group of affine transformations). Its action on $Z_p \otimes Z_p$ is given by

$$(\alpha_1,\alpha_2) \to (u_{11}\alpha_1 + u_{12}\alpha_2 + t_1, u_{21}\alpha_1 + u_{22}\alpha_2 + t_2). \tag{4.2}$$

The affine geometry of $Z_p \otimes Z_p$ is similar to that of an ordinary plane. A straight line passing through (α_1,α_2) and (α'_1,α'_2) is the set of p points:

$$\{(\alpha_1,\alpha_2) + a(\alpha'_1 - \alpha_1, \alpha'_2 - \alpha_2) | a = 0,1,...,p-1\}. \tag{4.3}$$

There are $p + 1$ lines passing through every point $Z_p \otimes Z_p$. An affine transformation maps each line into another line.

Let us call a straight line passing through the origin [the point (0,0)] a *ray.* Each ray is a Z_p subgroup of $Z_p \otimes Z_p$. There are no other subgroups of $Z_p \otimes Z_p$. Notice that GL(2, p) is a very large group as compared to $H_{Z_{pq}}$ or $H_{Z_{p^2}}$. Therefore we naively expect the automorphisms to play an even more important role here than in Secs. 2 and 3. This is indeed the case. In Ref. 2 we prove (relying on Schur's method and on a theorem from Ref. 6) that *for every* $Z_p \otimes Z_p$ *system the orbits of* G_0 *on* $Z_p \otimes Z_p$ *are given by a subgroup of* GL(2, p). The corresponding subgroup of Aff(2, p) is, however, not always a maximal symmetry group.

We can classify the automorphisms according to the number of rays left invariant (the number of eigenvectors in $Z_p \otimes Z_p$). An automorphism U belongs to one of the following types

(a) *U is a multiple of the unit matrix* ($p+1$ *eigenvectors*):

$$U=\begin{pmatrix} v & 0 \\ 0 & v \end{pmatrix}, \quad v\in \mathrm{GF}(p), v\neq 0. \tag{4.4}$$

There are $p-1$ automorphisms of this type. They form a cyclic group. This group is the center of GL(2, p), denoted C.

(b) *U is diagonalizable in* GF(p) (2 *eigenvectors*). Then there is a basis such that

$$U=\begin{pmatrix} v & 0 \\ 0 & w \end{pmatrix}, \quad v,w\in \mathrm{GF}(p),\ v\neq w\neq 0. \tag{4.5}$$

There are $1/2(p-2)(p-1)p(p+1)$ automorphisms of this type.

(c) *U can be brought to Jordan form* (*one eigenvectors*). Then there is a basis such that

$$U=\begin{pmatrix} v & 1 \\ 0 & v \end{pmatrix}, \quad v\in \mathrm{GF}(p), v\neq 0. \tag{4.6}$$

There are $(p-1)^2(p+1)$ automorphisms of this type.

(d) *The eigenvalue equation of U has no roots in* GF(p) (*no eigenvectors in* $Z_p\otimes Z_p$). This is similar to the case of a real matrix having complex eigenvalues. There are $1/2(p-1)^2p^2$ automorphisms of this type.

An automorphism can be seen as a permutation of the $p+1$ rays. All automorphisms of type (a) act as the unit permutation on the $p+1$ rays. The group GL(2, p)/C acts faithfully on the rays. In analogy with ordinary geometry, the set of rays is called the projective space $P(1,p)$ and GL(2, p)/C is called the projective group PGL(2, p).[5] The autormorphisms of type (b), (c), and (d) act as cyclic permutations of the $(p-1)$,(p),$(p+1)$ rays they do not fix. Any two cycles of the same type are related by a basis transformation.

Let us write $Z_p\otimes Z_p$ as a square tableau:

$$\begin{aligned} &(0,0),(1,0),\ldots,(p-1,0),\\ &(0,1),(1,1),\ldots,(p-1,1),\\ &\quad\cdot\quad\cdot\quad\cdot\quad\cdot\\ &(0,p-1),(1,p-1),\ldots,(p-1,p-1). \end{aligned} \tag{4.7}$$

As opposed to Eqs. (2.12) and (3.3) the tableau (4.7) is not unique. We can choose any of the $1/2p(p+1)$ pairs of rays as "system of coordinates." In analogy to Secs. 2 and 3, we divide the global symmetries of $Z_p\otimes Z_p$ systems into *three classes*. The proof that our list is complete will be given in Ref. 2.

Class 1: *G acts as a permutation group of both the rows and the columns of one of the tableaux* (4.7).

Let $v\in$GF(p) be as in Eqs. (2.8) and (2.8′). Define the group $H_{m,n;s}$ (both ms and ns divides $p-1$) as the group of diagonal matrices of the form

$$\begin{pmatrix} v^{[(p-1)/ms](is+r)} & 0 \\ 0 & v^{[(p-1)/ns](js+r)} \end{pmatrix} \tag{4.8}$$

$$i=1,\ldots,m;\ j=1,\ldots,n;\ r=1,\ldots,s.$$

TABLE III. The group GL(2,3).

Type	Length of cycle	Eigenvectors (as column!)	Matrices grouped in cycles
a	2	All	$\begin{pmatrix}1&0\\0&1\end{pmatrix}\begin{pmatrix}2&0\\0&2\end{pmatrix}$
b	2	$\begin{pmatrix}1\\0\end{pmatrix}$ and $\begin{pmatrix}0\\1\end{pmatrix}$	$\begin{pmatrix}1&0\\0&2\end{pmatrix};\begin{pmatrix}2&0\\0&1\end{pmatrix}$
		$\begin{pmatrix}1\\0\end{pmatrix}$ and $\begin{pmatrix}1\\1\end{pmatrix}$	$\begin{pmatrix}1&1\\0&2\end{pmatrix};\begin{pmatrix}2&2\\0&1\end{pmatrix}$
		$\begin{pmatrix}0\\1\end{pmatrix}$ and $\begin{pmatrix}1\\1\end{pmatrix}$	$\begin{pmatrix}2&0\\1&1\end{pmatrix};\begin{pmatrix}1&0\\2&2\end{pmatrix}$
		$\begin{pmatrix}0\\1\end{pmatrix}$ and $\begin{pmatrix}1\\2\end{pmatrix}$	$\begin{pmatrix}1&0\\1&2\end{pmatrix};\begin{pmatrix}2&0\\2&1\end{pmatrix}$
		$\begin{pmatrix}1\\0\end{pmatrix}$ and $\begin{pmatrix}1\\2\end{pmatrix}$	$\begin{pmatrix}2&1\\0&1\end{pmatrix};\begin{pmatrix}1&2\\0&2\end{pmatrix}$
		$\begin{pmatrix}1\\1\end{pmatrix}$ and $\begin{pmatrix}1\\2\end{pmatrix}$	$\begin{pmatrix}0&1\\1&0\end{pmatrix};\begin{pmatrix}0&2\\2&0\end{pmatrix}$
c	6	$\begin{pmatrix}1\\0\end{pmatrix}$	$\begin{pmatrix}1&1\\0&1\end{pmatrix}\begin{pmatrix}1&2\\0&1\end{pmatrix}\begin{pmatrix}2&1\\0&2\end{pmatrix}\begin{pmatrix}2&2\\0&2\end{pmatrix}$
		$\begin{pmatrix}0\\1\end{pmatrix}$	$\begin{pmatrix}1&0\\1&1\end{pmatrix}\begin{pmatrix}1&0\\2&1\end{pmatrix}\begin{pmatrix}2&0\\1&2\end{pmatrix}\begin{pmatrix}2&0\\2&2\end{pmatrix}$
		$\begin{pmatrix}1\\1\end{pmatrix}$	$\begin{pmatrix}0&1\\2&2\end{pmatrix}\begin{pmatrix}0&2\\1&1\end{pmatrix}\begin{pmatrix}2&2\\1&0\end{pmatrix}\begin{pmatrix}1&1\\2&0\end{pmatrix}$
		$\begin{pmatrix}1\\2\end{pmatrix}$	$\begin{pmatrix}0&1\\2&1\end{pmatrix}\begin{pmatrix}0&2\\1&2\end{pmatrix}\begin{pmatrix}1&2\\1&0\end{pmatrix}\begin{pmatrix}2&1\\2&0\end{pmatrix}$
d	8	None	$\begin{pmatrix}0&1\\1&1\end{pmatrix}\begin{pmatrix}1&1\\1&2\end{pmatrix}\begin{pmatrix}1&2\\2&0\end{pmatrix}\begin{pmatrix}0&2\\2&2\end{pmatrix}\begin{pmatrix}2&2\\2&1\end{pmatrix}\begin{pmatrix}2&1\\1&0\end{pmatrix}$
			$\begin{pmatrix}1&1\\1&0\end{pmatrix}\begin{pmatrix}2&1\\1&1\end{pmatrix}\begin{pmatrix}0&2\\2&1\end{pmatrix}\begin{pmatrix}2&2\\2&0\end{pmatrix}\begin{pmatrix}1&2\\2&2\end{pmatrix}\begin{pmatrix}0&1\\1&2\end{pmatrix}$
			$\begin{pmatrix}1&1\\2&1\end{pmatrix}\begin{pmatrix}0&2\\1&0\end{pmatrix}\begin{pmatrix}1&2\\1&1\end{pmatrix}\begin{pmatrix}2&2\\1&2\end{pmatrix}\begin{pmatrix}0&1\\2&0\end{pmatrix}\begin{pmatrix}2&1\\2&2\end{pmatrix}$

TABLE IV. The global symmetries of $Z_3 \otimes Z_3$ systems.

Global symmetry	Order of the group	Relations among the coupling constants
$Z_3 \otimes Z_3$	9	...
$M_{3\times 3}^{1,1;2}$	18	$b_{1,0}=b_{2,0}, b_{0,1}=b_{0,2}, b_{1,1}=b_{2,2}, b_{1,2}=b_{2,1}$
$M_{3\times 3}^{2,1;1}$	18	$b_{1,0}=b_{2,0}, b_{1,1}=b_{2,1}, b_{1,2}=b_{2,2}$
$S_3 \otimes S_3$	36	$b_{1,0}=b_{2,0}, b_{0,1}=b_{0,2}, b_{1,1}=b_{1,2}=b_{2,1}=b_{2,2}$
$S_3 \sim Z_2$	72	$b_{1,0}=b_{2,0}=b_{0,1}=b_{0,2}, b_{1,1}=b_{1,2}=b_{2,1}=b_{2,2}$
$Z_3 \sim Z_3$	81	$b_{0,1}=b_{1,1}=b_{2,1}, b_{0,2}=b_{1,2}=b_{2,2}$
$Z_3 \sim S_3$	162	$b_{0,1}=b_{0,2}=b_{1,1}=b_{2,2}=b_{1,2}=b_{2,1}$
$S_3 \sim Z_3$	648	$b_{1,0}=b_{2,0}, b_{0,1}=b_{1,1}=b_{2,1}, b_{0,2}=b_{1,2}=b_{2,2}$
$S_3 \sim S_3$	1296	$b_{1,0}=b_{2,0}, b_{0,1}=b_{0,2}=b_{1,2}=b_{2,1}=b_{1,1}=b_{2,2}$
S_9	9!	$b_{1,0}=b_{2,0}=b_{0,1}=b_{0,2}=b_{1,1}=b_{2,2}=b_{1,2}=b_{2,1}$

There are exactly $1/2p(p+1)$ different copies of $H_{m,n;s}$, one for each choice of the coordinate system (of course for a given basis in $Z_p \otimes Z_p$ only one of them consists of diagonal matrices).

Let us denote by $M_{p\times p}^{m,n;s}$ the corresponding subgroups of Aff(2, p). We have the following result.

For every symmetry of Class 1 the Lagrangian density is given by the orbits of one of the $H_{m,n;s}$ on $Z_p \otimes Z_p$. The corresponding maximal symmetry group is $G = M_{p\times p}^{m,n;s}$ except for the case $m = n = p-1, s = 1$ where $G = S_p \otimes S_p$ and $m \neq p-1, n = p-1$ when $G = M_p^m \sim S_p$.

Class 2: *G acts as a permutation group of only the rows (or only the columns) of one of the tableux* (4.7). The maximal symmetry groups of Class 2 are wreath products of a symmetry group of a Z_p system (M_p^m or S_p) acting inside each row (column) of (4.7) independently with a symmetry group of another Z_p system (M_p^n or S_p) acting as a permutation group of the rows (columns).

As opposed to symmetries of Class 1, there are only $p+1$ isomorphic copies of $M_p^m \sim M_q^n$, one for each ray. If G permutes the rows, the orbits of G_0 on $Z_p \otimes Z_p$ are determined via Eq. (4.2) by the subgroup of GL(2, p) containing $H_{m',n';s}$ (s is the largest divisor of m and n and we have $m's = m$ and $n's = n$) and the matrix

$$\begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}.$$

$H_{m',n';s}$ has to be chosen such that it maps the first row of (4.7) into itself. All other $p-1$ copies of $H_{m',n';s}$ which also map the first row into itself will be obtained as products of the original $H_{m',n';s}$ with powers of

$$\begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix}.$$

Class 3: *G does not preserve the row or the column structure of any of the tableaux* (4.7).

Let H be the subgroup of GL(2, p) that determines the orbits of G_0 on $Z_p \otimes Z_p$. We can divide the symmetries of Class 3 into two subclasses:

(a) *H is transitive on P*(1, p). *The corresponding maximal symmetry group is* $G = S_{p^2}$.

(b) *H is not transitive on P*(1, p). In this case there cannot be any automorphism of type c in H [if this were not true, then either H would be transitive on $P(1, p)$ or G would be of Class 2]. *H can be classified according to the lengths of its orbits in P*(1, p) (only the lengths of the orbits are important because we want to classify the symmetry groups up to basis transformations). *None of these orbits is allowed to contain only one ray* (if there is one orbit of length one, then G is of Class 2; if there is more than one orbit of length one, then G is of Class 1). A list of all subgroups of GL(2, P) is given in Ref. 5 so our problems is in principle solved. The details are, however, too technical and the interested reader can get them from Ref. 2.

If H is not transitive on P(1, p), *the maximal symmetry group is the subgroup of Aff*(2, p) *corresponding to H*, with one exception. If H is the group generated by $H_{p-1,p-1;1}$ [see Eq. (4.8)] and by the "flip matrix"

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

then the maximal symmetry group is $G = S_p \sim Z_2$ [one copy of S_p acts on the rows of (4.7), the second one on the columns and the Z_2 flips the rows into columns]. There are $1/2p(p+1)$ different copies of $S_p \sim Z_2$, one for each system of coordinates.

As an example, consider the $Z_3 \otimes Z_3$ systems. This is not the most typical example because there are only 4 rays. It is, however, instructive to compare the $Z_3 \otimes Z_3$ and Z_9 cases explicitly. GL(2,3) is of order 48 only, so we can give a complete list without the general results on the subgroups of GL(2, p). In Table III we give a list of the automorphisms of $Z_3 \otimes Z_3$ grouped according to their type, to the rays left invariant and to the cycles they form. In Table IV we give a list of the global symmetries. For symmetries which are related by a basis transformation we only give one representative.

It is interesting to compare Table II (Z_9) and Table IV ($Z_3 \otimes Z_3$). There are several cases when the two systems can be mapped into each other. This is the case of the $Z_3 \sim Z_3, Z_3 \sim S_3, S_3 \sim Z_3$, and $S_3 \sim S_3$ symmetries. But this does not include the $S_3 \otimes S_3$ or $S_3 \sim Z_2$ symmetries when the $Z_3 \otimes Z_3$ system factorizes (see I, Appendix B). Thus, contrary to our expectations there is no case when a Z_9 system factorizes. Such a factorization property was suggested by the Z_4 case.

Comparing Table I ($Z_2 \otimes Z_3$) and Table IV ($Z_3 \otimes Z_3$) one notices that the symmetry $S_3 \sim Z_2$ can occur on both manifolds.

Finally, let us explain the connection between G and $\tilde{G}$: the orbits of $\tilde{G}_0$ on $Z_p \otimes Z_p$ are given by the subgroup of GL(2, p) consisting of the transposes of the matrices of the subgroup of GL(2, p) that gives the orbits of G_0 on $Z_p \otimes Z_p$.

5. CONCLUSIONS

After this mathematical "tour de force" one can ask "What's next?" For the time being we do not intend to go further with our classification theory before we understand its physical implications. In further publications we will show how the standard group techniques can be applied for low and high temperature expansions. The methods used in these papers can also be used for Lagrangian functions depending on more than two variables (this includes lattice gauge theories). This will be the subject of a separate paper.

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On generalized torsion tensor fields and the reduced fiber bundle [a)]

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(Received 24 November 1980; accepted for publication 29 May 1981)

The reduction of a connection form ρ from a fiber bundle P to a subbundle Q is examined in detail; defining generalized torsion forms, we show how the usual Maurer–Cartan structural equations have to be modified. Examples and applications to classical general relativity and gauge theories are outlined.

PACS numbers: 02.20.Qs

I. INTRODUCTION

Fiber bundle techniques play an important role in gauge theories of physical fields as they give a geometrical meaning to the quantities involved in the formalism; furthermore, they provide an excellent framework for studying and solving problems of global and topological nature that surely would be much more difficult in other formalisms.

Gauge theories usually consider a given principal bundle $P = P(M,G)$ (M being the base manifold often identified with the space–time V^4, G the Lie structural group) and a connection ρ which, in turn, is interpreted as a physical field. Various arguments, essentially related to the problem of constructing a Lagrangian density, suggest considering also a preferred subgroup H of G, which is the true, unbroken group of symmetry of the theories. Examples may be found in the formulation of general relativity given by Trautman[1] and in the theory of McDowell and Mansouri,[2] as well as in the classical Maxwell and Yang–Mills gauge theories.

Mathematically the choice of H leads to the reduction of the bundle P to a subbundle $Q = Q(M,H)$,[3] thus giving rise to various problems, some of which are still open.

In Sec. II a theorem generalizing the classical concept of torsion tensor field for an arbitrary reduction $P \to Q$ is presented.

The most useful applications of these results may perhaps be found in gauge theories; nevertheless, in order to achieve a better understanding of the quantities involved, applications to general relativity, where there are no fundamental physical problems, are described in Sec. III.

Finally, in Sec. IV, we see that, at least formally, the method works also in the case of a graded Lie group. This is shown by deriving the structural equations in the McDowell–Mansouri theory.

II. THE MAIN THEOREMS

Let $P = P(M,G)$ be a principal fiber bundle over a manifold M with group G, and $Q = Q(M,H)$ a reduced subbundle of P with group H, a closed subgroup of G. Assume that the Lie algebra g of G admits a subspace f such that $g = h \oplus f$ and $\mathrm{ad}_h f \in f$. Using the following index convention, $i, j \in g$, $\alpha, \beta \in h$, $A, B \in f$, let ρ^i be a connection form in P with curvature $R^i = D_P \rho^i$ and $\mu^i = i^*(\rho^i)$, i being the injection of Q in P. Then we have

Theorem 1: (a) μ^α is a connection form in Q with curvature $\Omega^\alpha = D_h \mu^\alpha$;

(b) μ^A is a tensorial form on Q of type (ad, f) (i.e., $\mu^A \in \mathrm{hor}\Lambda^*(Q), R_a^* \mu^A = \mathrm{ad}(a^{-1})^A{}_B \mu^B$, $a \in H$);

(c) the connection form ρ^i is reducible to a connection form in Q if and only if $\mu^A = 0$;

(d) setting $\Theta = D_h \mu^A$ (2-forms of generalized torsion), the following generalized Maurer–Cartan structural equations (GMCSE) hold:

$$i^*(R^\alpha) = \Omega^\alpha + \tfrac{1}{2} C^\alpha{}_{AB} \mu^A \wedge \mu^B,$$

$$i^*(R^A) = \Theta^A + \tfrac{1}{2} C^A{}_{BC} \mu^B \wedge \mu^C,$$

Proof: (a) is verified by using the Proposition 6.4 of Ref. 3 (see p. 83). It is clear that $\Omega^\alpha = D_h \mu^\alpha = d\mu^\alpha + \tfrac{1}{2} C^\alpha{}_{\lambda\beta} \mu^\lambda \wedge \mu^\beta$.

(b) Defining D_i, the generators of g and D_i^*, as the fundamental vector fields associated with D_i in the fiber bundle P, we have $\rho(D_i^*) = D_i$ and then $\rho^A(D_\mu^*) = 0$. On the other hand, the field D_μ^* are i-related to field $D_\mu^*)_Q$ (the vector fields associated with the $D_\mu \in h$, in the bundle Q), and, therefore, for each $\mu \in Q$, we have $0 = \rho^A(i_*(D_\mu^*)_Q))$ $= (i^*(\rho^A))(D_\mu^*)_Q) = \mu^A(D_\mu^*)_Q)$. This implies that $\mu^A \in \mathrm{hor}\Lambda^*(Q)$. Furthermore, $R_a^* \rho^A = \mathrm{ad}(a^{-1})^A{}_B \rho^B + \mathrm{ad}(a^{-1})^A{}_\mu \rho^\mu$; the second term on the right side vanishes for the assumption on h and the injection of both sides now gives $R_a^* \mu^A = \mathrm{ad}(a^{-1})^A{}_B \mu^B$.

(c) is a trivial consequence of Proposition 6.4 of Ref. 3.

(d) is proved by straightforward calculation using the relations $R^\alpha = d\rho^\alpha + \tfrac{1}{2} C^\alpha_{ij} \rho^i \wedge \rho^j$, $R^A = d\rho^A + \tfrac{1}{2} C^A{}_{ij} \rho^i \wedge \rho^j$, the injection i^*, and the fact that $i^* d = d i^*$. Q.E.D.

Furthermore we have:

Theorem 2: Under the same assumption of theorem 1, by denoting $D = D_h$, we have

(a) $D\Omega^\alpha = 0$,

(b) $D\Theta^A + C^A{}_{B\lambda} \mu^B \wedge \Omega^\lambda = 0$.

Considering, respectively, a tensorial form of type (ad, h) and (ad, f) on Q, the following formulas hold:

(c) $DD\eta^\alpha = C^\alpha{}_{\mu\nu} \Omega^\mu \wedge \eta^\nu$, (d) $DD\eta^A = C^A{}_{\mu B} \Omega^\mu \wedge \eta^C$

Proof: (a), (b), (c) are trivial because μ^α is a connection form on Q. (d) follows from the general definition of covariant derivative for a tensorial form of type ρ: $DD\eta^A$

[a)]This work was carried out under the auspices of the National Group of Mathematical Physics of C.N.R.

0022-2488/81/122759-03$01.00

$= \rho^{A}{}_{B,\mu}(e)$. $\Omega^{\mu} \wedge \eta^{B}; \rho^{A}{}_{B,\mu}(e)$ are the "generators" of the representation ρ. In the actual case $\rho^{A}{}_{B,\mu}(e) = C^{A}{}_{B,\mu}$; then (d) follows. Q.E.D.

III. APPLICATIONS TO GENERAL RELATIVITY

(A) The first example is the well known reduction $P(M, A(n)) \to Q(M, \mathrm{GL}(n))$, here described only for completeness. The GMCSE are the usual structural equations $i^*(R^{ij}) = \Omega^{ij}$, $i^*(R^{i}) = d\omega^{i} + \omega^{i}{}_{k} \wedge \omega^{k}{}_{i}$, where $\omega^{i}{}_{k}$ is the h-component of the connection form $\rho^{i} = (\omega^{i}{}_{k}, \omega^{j})$ in P. Notice that ρ^{i} is never reducible (i.e., $\omega^{j} \neq 0$).

(B) Consider the reduction $P(M, A(n)) \to Q(M, \mathrm{O}(n))$. The subbundle Q exists if and only if the associated bundle $P/\mathrm{O}(n)$ admits a global section, that is, a field of symmetric $(n \times n)$ matrices and of 1-forms globally defined over M. The condition $\mathrm{ad}_{h} f \in f$ holds, where $f = R^{n} \oplus B$, B being the linear space of symmetric matrices. Denoting by $(\rho^{i}{}_{k}, \rho^{i})$ the connection form on P, $\mu^{ik} = i^*(\rho^{ik})$, $\mu^{i} = i^*(\rho^{i})$ and setting $\psi^{ij} = \mu^{(ij)}$, $\omega^{ij} = \mu^{[ij]}$, the GMCSE are

$$i^*(R^{[ij]}) = \Omega^{ij} + \psi^{i}{}_{k} \wedge \psi^{k}{}_{j}, \tag{3.1}$$

$$i^*(R^{(ij)}) = D\psi^{ij} \equiv \Theta^{ij}, \tag{3.2}$$

$$i^*(R^{i}) = D\mu^{i} + \psi^{i}{}_{k} \wedge \mu^{k} = \Theta_{i} + \psi^{i}{}_{k} \wedge \mu^{k}. \tag{3.3}$$

To clarify the geometrical meaning of Eqs. (3.1)–(3.3), let us restrict ourselves to linear connections (i.e., nongeneralized affine connections), making the choice $\mu^{i} = \omega^{i}, \omega^{i}$ being an orthonormal basis of the cotangent space (orthonormal with respect to $\eta_{ij} = \mathrm{diag}(-, +, +, +)$. The fields $T^{i} = i^*(R^{i})$ became the usual torsion 2-forms and, via the metricity of $\omega^{i}{}_{j}$, we have $D\eta_{ij} = 2\psi_{ij}$; the generalized 2-forms $(\Theta^{ij}, \Theta^{k})$ are the covariant derivatives of the couple (ψ^{ij}, ω^{k}). Clearly, ρ is never reducible to μ, but, whenever ψ^{ij} vanishes (i.e., is metric), ρ is reducible to a connection γ in the bundle $Q' = Q'(M, R^{n} \times \mathrm{O}(n))$. The system (3.1)–(3.3) is nothing but the resolution of a linear connection into its associated "classical torsion field" T^{i} and "no-metricity forms" $D\eta_{ij}$. If we introduce the Riemannian connection ψ_{ij}, and define $N_{ij} = \mu_{ij} - \psi_{ij}$, a simple calculation yields $T^{i} = N^{i}{}_{k} \wedge \omega^{k}$, $\psi^{ij} = Q^{(ij)}$, where $Q^{ij} = Q_{k}{}^{ij} \wedge \omega^{k}$, Q_{kij} being the no-metricity tensor explicitly given by

$$Q^{i}{}_{jk} = \tfrac{1}{2} g^{ir}(\nabla_{j} g_{rk} + \nabla_{k} g_{rj} - \nabla_{r} g_{jk}).$$

(C) Consider the reduction $P(V^4, A(4)) \to Q(V^4, \mathrm{SO}(3))$. Theorem 1, in this case, gives a simple, very compact, formalization of the theory of physical frame of reference in general relativity.[4] In this example we have

$$g = a(4), \quad h = \mathrm{so}(3), \quad f = R^{4} \oplus B(4) \oplus L,$$

where L is the homogeneous space $\mathrm{SO}(3,1)/\mathrm{SO}(3)$, that is, from a physical point of view, the Lobacewsky velocity space. In order to construct the reduction $P \to Q$ we need:

(i) a field of symmetric matrices,

(ii) a basis ω^{i} of the cotangent space,

(iii) a field of velocity λ_{0},

globally well defined over V^4. The field λ_{0} will be tangent to a congruence Γ whose lines (timelike in this example) are the world lines of physical observers.[5] In general, the GMCSE are quite cumbersome and not particulary enlightening; on the contrary, considering a metric, nongeneralized affine connection, setting $\rho = (\rho^{i}{}_{j}, \rho^{k})$ and $\omega = i^*(\rho)$, $\omega = (\omega^{i}{}_{j}, \omega^{k})$, we have

$$i^*(R^{[\mu\nu]}) = \Omega^{\mu\nu} + a^{\mu} \wedge a^{\nu}, \tag{3.4}$$

$$i^*(R^{(0\nu)}) = Da^{\nu}, \qquad \alpha, \mu, \cdots = 1,2,3, \tag{3.5}$$

$$i^*(R^{\mu}) = D\omega^{\mu} - a^{\mu} \wedge a^{0}, \tag{3.6}$$

$$i^*(R^{0}) = D\omega^{0} - a^{\mu} \wedge \omega^{\mu}, \tag{3.7}$$

where, in terms of the tetrad $(\lambda_{0}, \lambda_{\alpha})$ and of the dual base $(\omega^{0}, \omega^{\alpha})$, we have set $a^{\mu} = \omega^{0\mu}$. Here the metric tensor is η_{ij} and the fundamental form is $\Phi = \eta_{ij} \omega^{i} \otimes \omega^{j}$. Let us recall the following[4]:

Definition 3.1: A linear connection ∇ over V^4 is said adapted to Γ if:

(i) ∇ is a linear connection,

(ii) $\nabla \lambda_{0} = 0$,

(iii) $(\nabla v)^{\mu} = \nabla(v^{\mu})$, $v \in T(V^4)$ if $v = (v^{0}, v^{\mu})$.

Now we can state:

Theorem 3.1: The connection forms ω^{ij} realize the most general connection adapted to Γ.

Proof: It is an easy matter to verify that ω is adapted to Γ. To show the generality of ω, notice that the existence of Q provides a field λ_{0} and, through the metric, the form $\omega^{0} = -\Phi(\lambda_{0})$. On the contrary, there is no unique way of choosing the fields ω^{α}, every choice of which yields a "spatial soldering form". The observation that a^{μ} does not depend on the form ω^{μ}, the use of Eqs. (3.6)–(3.7) and the well-known theorem stating that a metric connection can be uniquely determined by its "classical torsion field" $i^*(R^{i})$ completes the proof. Q.E.D.

The field $D\omega^{\mu}$ is related in a very simple way to the "classical spatial and temporal torsion fields" Θ^{μ}, S. We leave the reader to verify the following:

$$\tilde{\Theta}^{\mu} = \langle D\omega^{\mu} | \lambda_{\nu} \wedge \lambda_{\alpha} \rangle \omega^{\nu} \wedge \omega^{\alpha},$$

$$\tilde{S} = \langle D\omega^{\mu} | \lambda_{\nu} \wedge \lambda_{0} \rangle \omega^{\nu} \wedge \omega^{\mu}.$$

Let us introduce the first order objects associated with Γ:

$\tilde{C} = \mathscr{L}_{\lambda_{0}}(\omega^{0})$ acceleration,

$\tilde{\Omega} = -2d\omega^{0} - 2\omega \wedge \tilde{C}$ spatial vortex tensor,

$\tilde{K} = \mathscr{L}_{\lambda_{0}}(\Phi) + 2\omega \odot \tilde{C}$ spatial deformation tensor of the congruence Γ.

Finally we have:

Theorem 3.2: Let ρ be the Riemannian connection $(R^{i} = 0)$; then $\tilde{\Theta} = 0$, $\tilde{S} = -\tilde{\Omega}$, $a^{\mu} = \tfrac{1}{2}(\tilde{K}^{\mu\nu} - \tilde{\Omega}^{\mu\nu})\omega^{\mu} + \tilde{C}^{\mu}\omega^{0}$.

The proof is straightforward using Eq. (3.6) and the definition of $\tilde{\Omega}$, $\tilde{K}$, $\tilde{C}$. The connection form ρ realizes for ω^{α} the Fermi–Walker transport law, that is, the ω^{α} are absolutely nonrotating.

IV. AN EXAMPLE AND RELATED PROBLEMS IN THE SUPERFIBER BUNDLE

Finally we check our results in a nonclassical application. Consider the McDowell–Mansouri gauge theory of supergravity; doing so, we have to study a fiber bundle with a graded structural group, namely, OSP (1,4). Obviously, we have to generalize our theorems to include in the formalism

anticommuting vectors in the algebra of the structural group. It is not easy to perform such a generalization in a rigorous way; on the other hand, it is possible to write down the GMCSE in a formal manner, insofar as they involve essentially only the graded Lie algebra of the group. In other words, the actual geometrical problem is the description of the graded manifold of the fiber; although some important results have been obtained (see among others, Ref. 6), the whole problem is still a matter of discussion (see Ref. 7 and the references therein).

However, bypassing these problems, we take into account a principal graded fiber bundle $P = P(V^4, \mathrm{OSP}(1,4))$ and its reduced subbundle $Q = Q(V^4, \mathrm{SL}(2C))$. The GMCSE

$$i^*(R^{ij}) = \tilde{\Omega}^{ij} - \omega^i \wedge \omega^j - \tfrac{1}{2} i \epsilon^{ijks} \bar{\xi} \sigma_{ks} \gamma_5 \wedge \xi,$$

$$i^*(R^{i}) = D\omega^i - \tfrac{1}{2} i \bar{\xi} \gamma^i \wedge \xi,$$

$$i^*(R) = D\xi + \tfrac{1}{2} i \omega^i \wedge \gamma_i \xi$$

are, directly, the equations obtained in Ref. 2, by means of which the expansion of the Lagrangian density $L = R^{ij} \wedge R^{ks} \epsilon_{ijks} + R\gamma_5 \wedge R$ gives (via a Wigner–Inönu contraction of OSP $(I, 4)$ the Lagrangian of supergravity.

Notice that the necessary (and sufficient) condition for the existence of Q now yields the global existence of a field OSP $(I, 4)/\mathrm{SL}(2C)$, that is, a field (ω^i, ξ). This point, together with theorem 1, ensures that ξ is a spinorial tensor form well defined over V^4 that can be used as a basis for the tangent superspace.

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Representations of the groups GL(n,R) and SU(n) in an SO(n) basis

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(Received 4 August 1980; accepted for publication 30 December 1980)

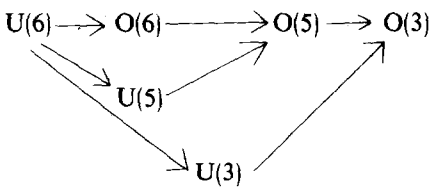
The explicit form for the infinitesimal operators and the (finite) matrix elements with respect to an SO(n) basis is obtained for the representations of the most degenerate series of the group SL(n,R), and for the irreducible unitary representations of the group SU(n) with highest weight (M,0,...,0).

PACS numbers: 02.20.Qs

1. INTRODUCTION

In this article *explicit* expressions are derived for the *infinitesimal operators*, and for the *finite matrix elements* of the group GL(n,R) for the case of its most degenerate series representations, and for the group U(n), for its unitary irreducible representations with highest weight (M,0,...,0) with respect to an SO(n) basis. As a consequence the corresponding representations are obtained also for the groups SL(n,R) and SU(n).

The groups SL(n,R) and SU(n), and their SO(n) subgroup, have found wide applications in physics. For example, applications of the group SU(n), making use of the SO(n) subgroup, are found both in the nuclear shell model[1] and in the atomic shell model.[2] The group–subgroups of these models which are relevant to the present article are SU($2j+1$) $\rightarrow$SO($2j+1$) and SU($2l+1$)$\rightarrow$SO($2l+1$), with j representing the total angular momentum and l the orbital angular momentum for single particles (nucleons, electrons). Another type of application is found in the harmonic oscillator model of nuclear forces where the group–subgroup relation U($3n$)$\rightarrow$O($3n$) is of relevance, with n representing the number of nucleons.[3] The case for $n=1$ corresponds to the familiar Elliott model.[4] More recently the interacting boson model of the nucleus has been developed,[5] based upon the quadrupole excitations of the liquid drop model by Bohr and Mottelson.[6] Adding to the five d-boson excitations an s-boson, the following (complete) symmetry chain has recently been investigated[7]:



This provides three examples of U(n)$\rightarrow$O(n) group–subgroup relationships. The six bosons transform according to the defining representation of U(6), and according to the (reducible) representation of O(3) with $l=2,0$ (l is the orbital angular momentum). Still another example is provided by a group theoretical formulation of band theory in solid state physics.[8] If n denotes the number of (equidistant) levels which are to be taken into account then, after a Bogoliubov transformation, the quasiparticles transform according to the group O($4n+1$). And again, in the symmetry chain that leads from O($4n+1$) to the physically relevant O(3) subgroup, the U(n)$\rightarrow$O(n) group–subgroup relation appears. Finally, the group–subgroup relationship SL(3,R)$\rightarrow$SO(3) has found applications in the theory of nuclear rotational bands,[9] in the quantum theory of general relativity,[10] and in particle physics.[11] A detailed analysis of SU(3)$\rightarrow$O(3) has been given in Ref. 12. The representations of the groups SL(3,R) and SL(n,R) have been discussed in Refs. 13 and 14, respectively.

In order to make use of symmetry considerations, it is essential to know, in explicit form, the infinitesimal operators of the group, as well as the representation matrix elements for the group elements themselves (which represent finite transformations). Different physical problems require in general different types of basis with respect to which the representations are to be determined. In Refs. 15 and 16 (see also Ref. 17) a method has been developed by means of which the infinitesimal operators and the finite matrix elements can be obtained for the compact semisimple Lie groups with respect to different choices of basis by making use of the principal nonunitary series representations. The possibilities that are admitted by this method are listed in Table I of Ref. 15a. In the following this method is used to determine the infinitesimal operators and the finite matrix elements for the representations of the group SU(n) [and SL(n,R)] in an SO(n) basis.

2. REPRESENTATIONS OF THE MOST DEGENERATE SERIES OF THE GROUP SL(n,R)

In the first part of this article we restrict our attention to the special linear group SL(n,R). The general linear group GL(n,R) will be considered later on.

The group SL(n,R) has a maximal compact subgroup which is isomorphic to SO(n). Let $G=ANK$ be an Iwasawa decomposition of SL(n,R).[18] We shall consider the representations of the most degenerate series of SL(n,R). They are induced by the representations of the maximal parabolic subgroup P_Θ, which can be represented as

$$P_\Theta = ANM_\Theta(K) = A_\Theta N_\Theta M_\Theta, \tag{1}$$

where the symbols A and N are the same as in the Iwasawa decomposition. For a description of the subgroups $A_\Theta, N_\Theta, M_\Theta$ and $M_\Theta(K)$, we refer to Ref. 18 or 17. The Iwasawa decomposition and the decomposition(1) can be

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 0022-2488/81/122762-08$01.00

chosen in such a manner that:

(a) A is represented by the subgroup [of SL(n,R)] that consists of all diagonal matrices with positive (real) elements.

(b) N is represented by the subgroup of all upper triangular matrices (with all matrix elements equal to 1 along the main diagonal).

(c) The group A_Θ is of the form $A_\Theta = \exp(t\alpha)$ with α a diagonal matrix of the form

$$\operatorname{diag}\left(\frac{-1}{n-1}, \frac{-1}{n-1}, \ldots, \frac{-1}{n-1}, 1\right). \tag{2}$$

(d) $M_\Theta(K)$ is represented by the subgroup $\mathrm{SO}(n-1)\otimes Z_2$ (Z_2 a cyclic group of order 2) and consists of the matrices

$$\operatorname{diag}(\mathrm{O}(n-1), \pm 1) \tag{3}$$

with the condition that the determinant is equal to 1.

(e) The subgroup M_Θ consists of the matrices

$$\operatorname{diag}(\mathrm{GL}(n-1,R), \pm 1) \tag{4}$$

with determinant equal to 1.

In the following it will be more convenient to consider representations of SL(n,R) that are induced from representations of the subgroup P_m rather than from the subgroup P_Θ. The subgroup P_m differes from P_Θ insofar as the subgroups of matrices given by Eqs. (3) and (4) are replaced by the subgroups $\mathrm{SO}(n-1)$ and $\mathrm{SL}(n-1,R)$, respectively [this amounts to disregarding the subgroup Z_2 in $M_\Theta(K)$ and in M_Θ]. The subgroup P_m then has the decomposition

$$P_m = AN\cdot\mathrm{SO}(n-1) = A_\Theta N_\Theta\cdot\mathrm{SL}(n-1,R).$$

The representations of SL(n,R) that are induced from the representations of P_m decompose into a direct sum of representations that are induced from representations of P_Θ. The precise nature of this decomposition can be obtained by considering the representation spaces.

We consider representations of SL(n,R) that are induced from one-dimensional representations of P_m:

$$hnm \to \exp[\lambda(\log h)], \quad h\in A_\Theta, n\in N_\Theta, m\in \mathrm{SL}(n-1,R). \tag{5}$$

Here λ is a linear form on the Lie algebra $\mathfrak{a}_\Theta$ of the Lie group A_Θ. Since $\mathfrak{a}_\Theta$ is one-dimensional the linear form λ is defined by one number. The representation π_λ of SL(n,R) which is induced by this representation of P_m can be realized on the Hilbert space $L^2_0(K)$, $K = \mathrm{SO}(n)$, of square integrable functions (with respect to an invariant measure on K) that satisfy the condition

$$f(mk) = f(k), \quad m\in\mathrm{SO}(n-1), \quad k\in\mathrm{SO}(n). \tag{6}$$

The action of the operators $\pi_\lambda(g)$ that represents the group element g on functions $f\in L^2_0(K)$ is given by

$$\pi_\lambda(g)f(k) = \exp[\lambda(\log h)]f(k_g), \tag{7}$$

where $h\in A_\Theta$ and $k_g\in K$ are defined in the following manner: k_g is defined by the Iwasawa decomposition $kg = h'nk_g$, $h'\in A$, $n\in N$; the element h' is uniquely decomposed into a product hh'' with $h\in A_\Theta$ [this is the h of Eq. (7)] and with $h''\in A(\Theta)$ [the group A is a direct product of its subgroups A_Θ and $A(\Theta)$]. For details see Ref. 18.

3. INFINITESIMAL OPERATORS FOR THE REPRESENTATIONS OF THE MOST DEGENERATE SERIES OF SL(n,R)

In order to evaluate the infinitesimal operators for the representations π_λ, Lemma 5.2 of Ref. 17 will be used (see also Ref. 15a). This lemma will be stated below.

Let $\mathfrak{g}$ denote the Lie algebra of SL(n,R). The commutative subalgebra $\mathfrak{a}_\Theta$ defines the system of restricted roots for the pair $(\mathfrak{g},\mathfrak{a}_\Theta)$ (see Ref. 18). Since $\mathfrak{a}_\Theta$ is one-dimensional, there exists only one simple restricted root. Let $B(\cdot,\cdot)$ be a Cartan–Killing form and θ a Cartan involution. Then $\langle x,y\rangle = -cB(x,\theta y)$, $c>0$ and fixed, is a scalar product on $\mathfrak{g}$. Let $\mathfrak{g} = \mathfrak{k} + \mathfrak{p}$ be a Cartan decomposition of $\mathfrak{g}$. The adjoint representation of $G = \mathrm{SL}(n,R)$ in $\mathfrak{g}$ will be denoted by Ad. Now Lemma 5.2 of Ref. 17 can be formulated as follows:

Lemma: The infinitesimal operators $d\pi_\lambda(Y)$, $Y\in\mathfrak{p}_c$ ($\mathfrak{p}_c$ the complexification of $\mathfrak{p}$), of the representation π_λ act upon the infinitely differentiable functions of $L^2_0(K)$ in the manner

$$\begin{aligned} d\pi_\lambda(Y)f(k) &= \langle(\mathrm{Ad}k)Y,H\rangle\lambda(H)f(k) - \langle(\mathrm{Ad}k)Y,\rho\rangle f(k) \\ &\quad + \tfrac{1}{2}[Q,\langle(\mathrm{Ad}k)Y,h\rangle]f(k), \end{aligned} \tag{8}$$

where H is a normalized element of $\mathfrak{a}_\Theta$, h is an element of $\mathfrak{a}_\Theta$ such that $\alpha(h) = 1$ [α is a simple restricted root of the pair $(\mathfrak{g},\mathfrak{a}_\Theta)$], Q is identical to the operator Q_1 of formula (5) of Ref. 15a, ρ is half the sum of the positive restricted roots of the pair $(\mathfrak{g},\mathfrak{a}_\Theta)$ (including multiple roots), and $[.,.]$ denotes the commutator.

For the space $L^2_0(K)$ an orthonormal basis is chosen in the following way. According to the Peter-Weyl theorem, the space $L^2(K)$ has a basis which consists of all the matrix elements of all nonequivalent irreducible representations of the group $K\equiv\mathrm{SO}(n)$. The elements of $L^2_0(K)$ satisfy the additional property given by Eq. (6). Thus a basis for the space $L^2(K)$ can be chosen which consists of all the matrix elements which are left invariant with respect to $\mathrm{SO}(n-1)$. The irreducible representation of $\mathrm{SO}(n)$ with highest weight

$$m\equiv(m_{1n},m_{2n},\ldots,m_{[n/2],n}), \quad m_{1n}\geqslant m_{2n}\geqslant\cdots$$

will be denoted by $D_m\equiv[m]$. Into the space of this representation we introduce two different orthonormal basis: the Gel'fand–Zetlin basis and another arbitrary, but fixed, orthonormal basis. The elements of this latter basis will be denoted by $|\Sigma\rangle$. The Gel'fand–Zetlin basis element that corresponds to the Gel'fand–Zetlin pattern

$$\begin{bmatrix} m_{1n} & \cdots & 0 & \cdots & 0 \\ & 0 & & 0 & \\ & & \ddots & \iddots & \\ & & & 0 & \end{bmatrix}, \tag{9}$$

where the first row is a highest weight of a representation D_m of $\mathrm{SO}(n)$, will be denoted by $|\Omega\rangle$ [i.e., the vector $|\Omega\rangle$ is invariant with respect to the subgroup $\mathrm{SO}(n-1)$]. It is obvious that a representation D_m has an $\mathrm{SO}(n-1)$-invariant vector if and only if its highest weight is of the form $(m_{1n},0,\ldots,0)$.

Now we consider the matrix elements of the form

$$(\dim[m])^{1/2}\langle\Omega|D_m(k)|\Sigma\rangle\equiv(\dim[m])^{1/2}D^m_{\Omega,\Sigma}(k),$$
$$k\in SO(n), m=(m_{1n},0,...,0). \tag{10}$$

The set of all such functions, for all $[m]$ and Σ, constitutes an orthonormal basis for $L^2_0(K)$. The Gel'fand–Zetlin pattern, Eq. (9), and thus the vector $|\Omega\rangle$, is determined by the representation $[m]$. The basis functions of Eq. (10) will henceforth be denoted by $|m,\Sigma\rangle$, where m denotes the integer m_{1n} of Eq. (9). The restriction of π_λ onto K acts on $L^2_0(K)$ according to $\pi_\lambda(k_0)f(k)=f(kk_0)$. Therefore, $\pi_\lambda|_K$ does not change the value of m in $|m,\Sigma\rangle$. The irreducible representations $[m]$ of $K\equiv SO(n)$ are contained in π_λ not more than once. Moreover, $\pi_\lambda|_K$ contains all irreducible representations of $SO(n)$ with highest weight $[m]=(m_{1n},0,...,0)$, and only these.

Now we use formula (8) in order to derive an explicit expression for the infinitesimal operators $d\pi_\lambda(Y)$ in the basis $|m,\Sigma\rangle$. The derivation is similar to the one given in Ref. 15a for the representations of the groups $U(p,q)$. Therefore, we omit here the details.

The Cartan involution θ in $\mathfrak{g}$ is given as $\theta(X)=-X^T$. Therefore,

$$\langle X,Y\rangle=\mathrm{Tr}XY^T, \tag{11}$$

where T denotes a transposition. Then the matrix

$$H=\frac{1}{[n(n-1)]^{1/2}}\left[\sum_{j=1}^{n-1}e_{jj}-(n-1)e_{nn}\right] \tag{12}$$

is a normalized element in $\mathfrak{a}_\Theta$. Here e_{ij} is a matrix with matrix elements $(e_{ij})_{st}=\delta_{is}\delta_{jt}$. The simple restricted root α of the pair $(\mathfrak{g},\mathfrak{a}_\Theta)$ is given by

$$\alpha[e_{nn}-(1/n)(e_{11}+\cdots+e_{nn})]=1. \tag{13}$$

Hence the h of the lemma is given by

$$h=[(n-1)/n]e_{nn}-(1/n)(e_{11}+\cdots+e_{n-1,n-1}). \tag{14}$$

The formula $\alpha(h')=\langle h_\alpha,h'\rangle$, $h'\in\mathfrak{a}_\Theta$, defines the correspondence between α and the element $h_\alpha\in\mathfrak{a}_\Theta$. It is easily found that

$$h_\alpha=e_{nn}-[1/(n-1)](e_{11}+\cdots+e_{n-1,n-1}). \tag{15}$$

It is also easy to verify that

$$\langle \mathrm{Ad}k)Y,H\rangle\lambda(H)=\langle \mathrm{Ad}k)Y,h\rangle\lambda(h_\alpha) \tag{16}$$

and

$$\langle(\mathrm{Ad}k)Y,\rho\rangle=\tfrac{1}{2}(p+2q)\langle\alpha,\alpha\rangle\langle(\mathrm{Ad}k)Y,h\rangle, \tag{17}$$

where p is the multiplicity of the root α and q the multiplicity of the root 2α. In our case $p=n-1, q=0$. Since we consider the degenerate series of representations, the chain (2) of subgroups of Ref. 15a reduces to

$$SO(n)=K\equiv K_1\supset K_2\equiv SO(n-1).$$

Moreover, the chain of subgroups (3) of Ref. 15a reduces to the same two subgroups, i.e., there are no subgroups between $SO(n-1)$ and $SO(n)$. This information is utilized to define the operator Q [see Eq. (5) of Ref. 15a]. The operator Q acts upon the state $|m,\Sigma\rangle$ as

$$Q|m,\Sigma\rangle=q(m)|m,\Sigma\rangle. \tag{18}$$

According to Eq. (16)–(18) it follows that

$$d\pi_\lambda(Y)|m,\Sigma\rangle$$
$$=\{\langle\lambda,\alpha\rangle-[(n-1)/2]\langle\alpha,\alpha\rangle+\tfrac{1}{2}[Q-q(m)]\}$$
$$\times\langle(\mathrm{Ad}k)Y,h\rangle|m,\Sigma\rangle. \tag{19}$$

The expression $\langle(\mathrm{Ad}k)Y,h\rangle|m,\Sigma\rangle$ is evaluated as follows. For the elements $Y\in\mathfrak{p}$ we take the basis elements of $\mathfrak{p}$. The space $\mathfrak{p}$ forms the carrier space for an irreducible representation of the subalgebra $so(n)$ with respect to the action $\mathrm{ad}b$, $b\in so(n)$. We choose in $\mathfrak{p}$ a Gel'fand–Zetlin basis (i.e., a basis such that the representation is given by the Gel'fand–Zetlin formulas). The space $\mathfrak{p}$ is the carrier space of the irreducible representation of $so(n)$ with highest weight $(2,0,...,0)$ and the Gel'fand–Zetlin basis coincides with

$$I_{ij}=e_{ij}+e_{ji},\quad i<j,$$
$$I_{ii}=e_{ii}-\frac{1}{n}\left(\sum_{j=1}^{n}e_{jj}\right),\quad i=2,3,...,n.$$

The correspondence with the Gel'fand–Zetlin patterns is then

$$I_{j-k,j}\longleftrightarrow \begin{matrix} \\ n-j+1\{ \\ \\ k\{ \\ \\ \\ \\ \\ \end{matrix}\begin{bmatrix} 2 & 0 & \cdot & \cdot & \cdot & \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot & & \cdot & & \cdot & \cdot \\ 2 & & 0 & \cdot & \cdot & \cdot & 0 & \\ & 1 & & 0 & \cdot & \cdot & \cdot & \\ & & \cdot & & \cdot & \cdot & \cdot & \\ & & & 1 & & 0 & \cdot\cdot & \\ & & & & 0 & & \cdot\cdot & \\ & & & & & \cdot & \cdots & \\ & & & & & & 0 & \end{bmatrix}, \tag{20}$$

$$j=1,2,...,n,\quad k=0,1,...,j.$$

Since, for $b\in so(n)$, one has

$$(\mathrm{ad}b)I_{ii}=(\mathrm{ad}b)e_{ii}, \tag{21}$$
$$(\mathrm{ad}b)h=[(n-1)/n](\mathrm{ad}b)e_{nn}, \tag{22}$$

it follows that

$$\langle \mathrm{Ad}k)I_{jj},h\rangle=[(n-1)/n]\langle(\mathrm{Ad}k)e_{jj},e_{nn}\rangle, \tag{23}$$
$$\langle(\mathrm{Ad}k)I_{sj},h\rangle=[(n-1)/n]\langle(\mathrm{Ad}k)I_{sj},e_{nn}\rangle,\quad s<j. \tag{24}$$

Since $(\mathrm{Ad}k)I_{sj},e_{nn}\rangle$ is the matrix element $D^{\{2\}}_{(e_{nn}),(I_{sj})}(k)$ of the representation $\{2\}$ with highest weight (2,0,...,0) we have, due to Eq. (10) [here (e_{nn}) and (I_{sj}) denote the vectors that correspond to the appropriate Gel'fand–Zetlin pattern of Eq. (20)]:

$$\begin{aligned}&\langle(\mathrm{Ad}k)I_{sj},e_{nn}\rangle|m,\Sigma\rangle\\&\quad=(\dim[m])^{1/2}D^{\{2\}}_{(e_{nn}),(I_{sj})}(k)D^{m}_{\Omega,\Sigma}(k)\\&\quad=\sum_{m',\Sigma'}(\dim[m]/\dim[m'])^{1/2}\langle[m']\Omega;\{2\},(e_{nn})|[m'],\Omega\rangle\\&\quad\times\langle[m'],\Sigma'|[m],\Sigma;\{2\},(I_{sj})\rangle|m',\Sigma'\rangle,\end{aligned}\tag{25}$$

where $\langle\cdots;\cdots|\cdots\rangle$ and $\langle\cdots|\cdots;\cdots\rangle$ are Clebsch–Gordon coefficients (CGc) for SO(n). The first CGc is taken for the Gel'fand–Zetlin basis, the second CGc for the basis $|m,\Sigma\rangle$, which may differ from the Gel'fand–Zetlin basis. The summation in Eq. (25) is over all vectors $|m',\Sigma'\rangle$ for which the second CGc is not equal to zero.

Because of the properties of the CGc the tensor product $[m,0,...,0]\otimes\{2\}$ in Eq. (25) decomposes into a direct sum of irreducible representations:

$$\begin{aligned}&[m,0,...,0]\otimes\{2\}=[m+2,0,...,0]\oplus[m-2,0,...,0]\\&\quad\oplus[m,2,0,...,0]\oplus[m+1,1,0,...,0]\oplus[m-1,1,0,...,0]\\&\quad\oplus[m,0,...,0].\end{aligned}\tag{26}$$

This decomposition is valid as it stands for $m\geqslant 2$. For $m<2$ the terms that do not satisfy the dominant weight condition $m_{1n}\geqslant m_{2n}\geqslant\cdots$ must be deleted.

In the restriction $\pi_\lambda|_{\mathrm{SO}(n)}$ only representations of SO(n) occur which have highest weights $(m,0,...,0)$. Thus in Eq. (26) it is only the representations $[m+2,0,...,0]$, $[m-2,0,...,0]$, and $[m,0,...,0]$ that are of relevance and thus the values of m' in Eq. (25) are restricted to $m'=m+2,\ m-2,\ m$. Now Eq. (19) is considered. The number $\langle\lambda,\alpha\rangle\equiv\lambda(h_\alpha)$ will be denoted by σ. Then the following relation holds:

$$[(n-1)/2]\langle\alpha,\alpha\rangle=[(n-1)/2]\langle h_\alpha,h_\alpha\rangle=n/2.\tag{27}$$

The decomposition given by Eq. (25) is now applied to $\langle(\mathrm{Ad}k)Y,h\rangle|m,\Sigma\rangle$. The operator $[Q-q(m)]/2$, acting from the left on the sum in Eq. (25), yields the number $[q(m')-q(m)]/2$. This number is evaluated for $m'=m\pm 2$ (either directly, or by utilizing the considerations given in Sec. 4 of Ref. 15a). The formula for the action of the infinitesimal operators $d\pi_\lambda(I_{sj})$ of the representation π_λ of SL(n,R) in an SO(n) basis is then obtained as

$$\begin{aligned}d\pi_\lambda(I_{sj})|m,\Sigma\rangle&=\frac{n-1}{n}(\sigma+m)\left(\frac{\dim[m]}{\dim[m+2]}\right)^{1/2}\sum_{\Sigma'}\langle[m],\Omega;\{2\},(e_{nn})|[m+2],\Omega\rangle\langle[m+2],\Sigma'|[m],\Sigma;\{2\},(I_{sj})\rangle|m+2,\Sigma'\rangle\\&+\frac{n-1}{n}(\sigma-m-n+2)\left(\frac{\dim[m]}{\dim[m-2]}\right)^{1/2}\sum_{\Sigma'}\langle[m],\Omega;\{2\},(e_{nn})|[m-2],\Omega\rangle\langle[m-2],\Sigma'|[m],\Sigma;\{2\},(I_{sj})\rangle|m-2,\Sigma'\rangle\\&+\frac{n-1}{n}\left(\sigma-\frac{n}{2}\right)\sum_{\Sigma'}\langle[m],\Omega;\{2\},(e_{nn})|[m],\Omega\rangle\langle[m],\Sigma'|[m],\Sigma;\{2\},(I_{sj})|m,\Sigma'\rangle.\end{aligned}\tag{28}$$

This formula expresses the infinitesimal operators with the help of CGc of the group SO(n) for the tensor product $[m,0,...,0]\otimes[2,0,...,0]$. These CGc will be evaluated for various types of basis in another article.

The infinitesimal operators $d\pi_\lambda(I_{sj})$ change the number m by ± 2, or they leave m unchanged. Thus they leave invariant the subspace that is spanned by the vectors $|m,\Sigma\rangle$ with m odd and the subspace that is spanned by the vectores $|m,\Sigma\rangle$ for which m is even. On these subspaces representations of SL(n,R) are realized that are induced by the one-dimensional representation of the subgroup P_Θ. These are, for the case of even m the representation π_σ^+ of SL(n,R), induced from the representation

$$hnm\rightarrow\exp[\lambda(\log h)],\quad h\in A_\Theta,\ n\in N_\Theta,\ m\in M_\Theta,\tag{29}$$

of P_Θ, and for the case of odd m the representation π_σ^- of SL(n,R), induced from the representation

$$\begin{aligned}&hnm'z\rightarrow\exp[\lambda(\log h)]\delta(z),\\&h\in A_\Theta,\ n\in N_\Theta,\ m'\in\mathrm{SL}(n-1,R),\ z\in Z_2,\end{aligned}\tag{30}$$

of P_Θ. Here $\delta(z)$ is a nontrivial representation of Z_2 [i.e., $\delta(z)\neq 1$, for $z\neq e$, the identity], and $\sigma=\lambda(h_\alpha)$.

4. THE STRUCTURE OF THE REPRESENTATIONS π_σ^+, π_σ^-

The multiplicity of the irreducible representations of the subgroup SO(n) in π_σ^+ and π_σ^- does not exceed 1. Moreover, the explicit form for the infinitesimal operators $d\pi_\sigma^\pm(Y)$, $Y\in\mathfrak{p}$, is known. Thus it is possible to determine the subset of irreducible representations from among the set of representations $\pi_\sigma^+,\pi_\sigma^-,\sigma$ a complex number, and to investigate the structure of the reducible representations $\pi_\sigma^+,\pi_\sigma^-$. The procedure to be followed is completely analogous to the one which was followed in Ref. 17 for the case of the groups U(n,1) and SO$_0$(n,1). Thus we list here merely the theorems without giving proofs. It will be easy for the reader to obtain the proofs by following the proofs given in Ref. 17.

Theorem 1: The representation π_σ^+ is completely irreducible if and only if $\sigma\neq 0,-2,-4,-6,\cdots$ and $\sigma\neq n,n+2,n+4,\cdots$. The representation π_σ^- is completely irreducible if and only if $\sigma\neq -1,-3,-5,\cdots$ and $\sigma\neq n+1,n+3,n+5,\cdots$.

Theorem 2: *If* $\sigma=p,p=0,-2,-4,\cdots$, then $\pi_\sigma^+\equiv\pi_p^+$ contains two completely irreducible representations of SL(n,R): a finite-dimensional representation D_{-p} with highest weight $(-p,0,...,0)$ and an infinite-dimensional representation, denoted by D^d_{-p+2}. The representation π_p^+ is not completely reducible (i.e., it is indecomposable) and the finite-dimensional representation is realized on the invariant subspace. Under restriction to the subgroup SO(n) the finite-dimensional representation D_{-p} decomposes into a direct sum of SO(n) irreducible representations with highest weights $(q,0,...,0)$ $q=0,2,4,...,-p$. The representation D^d_{-p+2} decomposes into a direct sum of SO(n) irreducible

representations with highest weights $(q,0,\ldots,0)$, $q = -p+2, -p+4, -p+6, \cdots$. If $\sigma = p'$, $p' = n, n+2, n+4, \cdots$, then the representation $\pi^{+}_{p'}$ is indecomposable and contains two completely irreducible representations of $SL(n,R)$, namely the finite-dimensional representation $D_{p'-n}$ with highest weight $(p'-n,0,\ldots,0)$ and the infinite-dimensional representation $D^{d}_{p'-n+2}$, which is realized on the invariant subspace. Thus the representations π^{+}_{p} and π^{+}_{n-p}, $p = 0, -2, -4, \cdots$, contains the same completely irreducible representations of $SL(n,R)$.

Theorem 3: If $\sigma = p, p = -1, -3, -5, \cdots$, then the representation $\pi^{-}_{\sigma} = \pi^{-}_{p}$ is indecomposable and contains two completely irreducible representations of $SL(n,R)$: the finite-dimensional representation D_{-p} with highest weight $(-p,0,\ldots,0)$ and the infinite-dimensional representation D^{d}_{-p+2}. The representation D_{-p} decomposes into a direct sum of $SO(n)$ irreducible representations with highest weights $(q,0,\ldots,0)$ $q = 1,3,5,\ldots, -p$ and D^{d}_{-p+2} decomposes into a direct sum of $SO(n)$ irreducible representations with highest weights $(q,0,\ldots,0)$, $q = -p+2, -p+4, -p+6, \cdots$. The representation D_{-p} is realized on the invariant subspace. If $\sigma = p'$, $p' = n+1, n+3, n+5, \cdots$. Then the representation $\pi^{-}_{p'}$ is indecomposable and contains the same completely irreducible representations of $SL(n,R)$ as $\pi^{-}_{n-p'}$, but now the infinite-dimensional representation is realized on the invariant subspace.

The representations $\pi^{\pm}_{i\tau+n/2}$, $i = (-1)^{1/2}$ and τ a real number, form the *principal most degenerate unitary series* of representations of $SL(n,R)$.

5. INFINITESIMAL OPERATORS FOR THE UNITARY REPRESENTATIONS OF THE GROUP SU(n) IN AN SO(n) BASIS

Consider the finite-dimensional representations of $SL(n,R)$ which are contained in the reducible representations π^{+}_{σ} (see Sec. 4). The Lie algebra of $SL(n,R)$ has the Cartan decomposition

$$\mathfrak{g} = \mathfrak{k} + \mathfrak{p}, \quad \mathfrak{k} = so(n).$$

The corresponding compact Lie algebra su(n) [the Lie algebra of the group SU(n)] has then the Cartan decomposition

$$\mathfrak{g} = \mathfrak{k} + (-1)^{1/2}\mathfrak{p}. \tag{31}$$

Hence, by multiplying the infinitesimal operators $Y \in \mathfrak{p}$ of the finite dimensional representations of $SL(n,R)$ by $(-1)^{1/2}$, one obtains the infinitesmial operators $X = (-1)^{1/2}Y \in (-1)^{1/2}\mathfrak{p}$ for the finite-dimensional representations of $SU(n)$. Thus Eq. (28) gives, after multiplication by $(-1)^{1/2}$, for $\sigma = 0, -1, -2, -3, \cdots$, the infinitesimal operators $J_{sj} = (-1)^{1/2}I_{sj}$ for the finite-dimensional representations of $SU(n)$ with highest weights $(-\sigma,0,\ldots,0)$ in an $SO(n)$ basis. These infinitesimal operators do, however, not satisfy the unitary condition $J^{*}_{sj} = -J_{sj}$. In order to obtain infinitesimal operators which satisfy the unitarity condition, it is necessary to introduce a new basis. The new basis elements $|m,\Sigma\rangle'$ are defined, for the finite-dimensional representations with highest weights $(-\sigma,0,\ldots,0)$, σ even, by

$$|m,\Sigma\rangle = (\lambda^{+}_{m})^{1/2}|m,\Sigma'\rangle, \tag{32}$$

with

$$\lambda^{+}_{0} = 1, \quad \lambda^{+}_{m} = \prod_{j=0}^{(m-2)/2} \frac{n-\sigma+2j}{\sigma+2j}, \tag{33}$$

and for the finite-dimensional representations with highest weights $(-\sigma,0,\ldots,0)$, σ odd, by

$$|m,\Sigma\rangle = (\lambda^{-}_{m})^{1/2}|m,\Sigma\rangle', \tag{34}$$

with

$$\lambda^{-}_{0} = 1, \quad \lambda^{-}_{m} = \prod_{j=0}^{(m-3)/2} \frac{n-\sigma+2j+1}{\sigma+2j+1}. \tag{35}$$

Note that the expressions (33) and (35) are the matrix elements of the intertwining operators for the representations $\pi^{\pm}_{\sigma}$ and $\pi^{\pm}_{n-\sigma}$ (see Refs. 16 and 17). For the representations $\pi^{+}_{i\tau+n/2}$ of the principal most degenerate unitary series an analogous introduction of a new basis will also lead to representations by unitary matrices (i.e., to skew-Hermitian infinitesimal operators).

In the new basis $|m,\Sigma\rangle'$, introduced by Eqs. (32)–(35), the following expression is obtained for the infinitesimal operators J_{sj} of the finite dimensional $SU(n)$ representations with highest weights $(M,0,\ldots,0)$ in an $SO(n)$ basis,

$$\begin{aligned} J_{sj}|m,\Sigma\rangle' = \frac{n-1}{n}\{ &-[(M-m)(M+m+n)]^{1/2}\left(\frac{\dim[m]}{\dim[m+2]}\right)^{1/2}\sum_{\Sigma'}\langle[m],\Omega;\{2\},(e_{nn})|[m+2],\Omega\rangle \\ &\times\langle[m+2],\Sigma'|[m],\Sigma;\{2\},(I_{sj})\rangle|m+2,\Sigma'\rangle' + [(M-m+2)(M+m+n-2)]^{1/2}\left(\frac{\dim[m]}{\dim[m-2]}\right)^{1/2} \\ &\times\sum_{\Sigma'}\langle[m],\Omega;\{2\},(e_{nn})|[m-2],\Omega\rangle\langle[m-2],\Sigma'|[m],\Sigma;\{2\},(I_{sj})\rangle|m-2,\Sigma'\rangle' \\ &-(-1)^{1/2}\left(M+\frac{n}{2}\right)\sum_{\Sigma'}\langle[m],\Omega;\{2\},(e_{nn})|[m],\Omega\rangle\langle[m],\Sigma'|[m],\Sigma;\{2\},(I_{sj})\rangle|m,\Sigma'\rangle'\}. \end{aligned} \tag{36}$$

The matrices J_{sj} in the basis $|m,\Sigma\rangle'$ satisfy the unitary condition $J^{*}_{sj} = -J_{sj}$.

6. MATRIX ELEMENTS FOR THE REPRESENTATIONS OF THE PRINCIPAL MOST DEGENERATE SERIES OF GL(n,R) IN AN SO(n) BASIS

It will be more convenient to consider in this section the group $GL(n,R)$ rather than the group $SL(n,R)$. The group $GL(n,R)$ is isomorphic to the direct product of the group $SL(n,R)$ and the group of all real numbers, excluding zero, with ordinary multiplication as group operation. The connected component of this group of real numbers will be denoted by R_0. The group $GL(n,R)$ consists of two disjoint pieces, with $\det g > 0$ and $\det g < 0$. Here we consider only the connected subgroup of $GL(n,R)$, and in what follows $GL(n,R)$, will denote the connected subgroup. The Iwasawa

decomposition for GL(n,R) is of the form $G = A'NK$, where $A' = AR_0$. [A is a component of the Iwasawa decomposition of SL(n,R) and N,K are the same as for the group SL(n,R).] We consider the space $L_0^2(K)$, which was introduced in Sec. 2, and induce on it a representation of GL(n,R) from the one-dimensional representation of the subgroup $P = A'N \cdot SO(n-1) \equiv R_0 P_m \equiv R_0 A_\Theta N_\Theta \cdot SL(n-1,R)$. The group R_0 can be identified with the subgroup of GL(n,R) that consists of the diagonal matrices

$$\text{diag}(s,s,\ldots,s) \quad s>0. \tag{37}$$

The subgroup A_Θ consists of the diagonal matrices

$$\text{diag}(t,t,\ldots,t,t^{-(n-1)}), \quad t>0. \tag{38}$$

It follows from Eqs. (37), (38) that the subgroup R_0A_Θ can be represented as a product A_1A_2, where A_1 consists of the matrices

$$\text{diag}(s,s,\ldots,s,1), \quad s>0, \tag{39}$$

and A_2 consists of the matrices

$$\text{diag}(1,1,\ldots,1,t), \quad t>0. \tag{40}$$

We consider the one-dimensional representation of the group $P = R_0A_\Theta N_\Theta \cdot SL(n-1) = A_1A_2N_\Theta \cdot SL(n-1,R)$ given by

$$h_1h_2nm \to \exp[\mu(\log h_2)],$$
$$h_1 \in A_1, h_2 \in A_2, \; n \in N_\Theta, \; m \in SL(n-1,R). \tag{41}$$

The linear form μ on the Lie algebra $\mathfrak{a}_2$ of A_2 is defined by one number. We denote this number also by μ in view of the fact that $\exp[\mu(\log h_2)] = t^\mu$, with t representing the element h_2 as given by Eq. (40). The operators of the representation of GL(n,R) that is induced by the representation of the group P, Eq. (41), on the space $L_0^2(K)$ is given by the formula

$$\pi_\mu(g)f(k) = \exp[\mu(\log h_2)]f(k_g), \tag{42}$$

where h_2 and k_g are defined in the following manner: The elements g of $G = A'NK = A_1A_2NK$ can be uniquely decomposed into a product of elements of A_1, A_2, N, and K. Thus we have the unique decomposition $kg = h_1h_2nk_g$, $h_1 \in A_1$, $h_2 \in A_2$, $n \in N$, $k_g \in K$. The elements h_2 and k_g of Eq. (42) are uniquely defined by this decomposition.

By decomposing the group GL(n,R) into the direct product SL(n,R) $\otimes$ R_0, it is easy to see that the representation π_μ of GL(n,R) decomposes into the product of the representations $\pi_{-\mu}$ of SL(n,R) [see Eq. (7)] and a one-dimensional representation of R_0. This fact will be needed in what follows.

In order to obtain the matrix elements of the representation π_μ of GL(n,R) in the SO(n) basis, an orthonormal basis has to be introduced into $L_0^2(K)$. In this basis the matrix elements

$$\int \overline{f_1(k)}\,[\pi_\mu(g)f_2(k)]dk \tag{43}$$

need to be evaluated, where $f_1(k), f_2(k)$ are orthonormal basis elements of $L_0^2(K)$ and dk is an invariant measure on SO(n). We proceed as follows: The group elements $g \in$ GL(n,R) can be decomposed into a product

$$g = k'hk, \quad k,k' \in SO(n), \; h \in A' \equiv AR_0. \tag{44}$$

The matrix elements for the representations of SO(n) with highest weight $(m,0,\ldots,0)$ in the Gel'fand–Zetlin basis are known.[19] [The expression for the matrix elements as given in Ref. 19 contains an integral. However, the matrix elements for the representations of the group $SO_0(n,1)$ in the Gel'fand–Zetlin basis, given in Ref. 20, can be utilized to obtain the matrix elements for the representations of the group SO($n+1$). For details see Ref. 16.] Thus we actually need to evaluate merely the matrix elements for the operators $\pi_\mu(h)$, $h \in A'$. According to Eq. (44) the matrix elements for the operators $\pi_\mu(g)$ can be represented as a finite sum of products of matrix elements for the operators $\pi_\mu(h)$ and of matrix elements for irreducible representations of SO(n).

Since

$$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & t \end{pmatrix}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \begin{pmatrix} t & 0 \\ 0 & 1 \end{pmatrix}, \tag{45}$$

we have to evaluate matrix elements for the operators $\pi_\mu(a_t)$, where

$$a_t = \text{diag}(1,1,\ldots,1,t), \quad t>0. \tag{46}$$

The matrix elements of the operator $\pi_\mu(a_t')$, where

$$a_t' = \text{diag}(1,1,\ldots,1,t,1,\ldots,1), \tag{47}$$

are obtained from the matrix elements of the operator $\pi_\mu(a_t)$ and the matrix elements of the operators $\pi_\mu(r)$ $\pi_\mu(r^{-1})$, where r and r^{-1} are elements of SO(n) that affect a permutation of the matrix element t of a_t along the diagonal [analogous to Eq. (45)]. Thus the matrix elements for the operator $\pi_\mu(a_t)$ need to be evaluated, where a_t is of the form of Eq. (46).

According to Eq. (6) the functions of $L_0^2(K)$ can be considered as functions on the sphere $S^{n-1} = SO(n-1) \backslash SO(n)$. In order to introduce a parametrization on S^{n-1}, we consider the parametrization of the elements g of SO(n) with the help of the decomposition

$$g = k'g_{n,n-1}(\theta_1)g_{n-1,n-2}(\theta_2)\cdots g_{21}(\theta_{n-1}), \tag{48}$$

where $k' \in SO(n-1)$ and $g_{jj-1}(\theta)$ is a rotation in the plane $(jj-1)$ about an angle θ (see Chap. 1 of Ref. 19). Then $\theta_1, \theta_2, \ldots, \theta_{n-1}$ provide a parametrization on S^{n-1}. The functions of $L_0^2(K)$ can thus be considered as functions $f(\theta_1,\theta_2,\ldots,\theta_{n-1})$. Now we define the action of $\pi_\mu(a_t)$ on these functions. We have

$$g_{n,n-1}(\theta_1)g_{n-1,n-2}(\theta_2)\cdots g_{21}(\theta_{n-1})a_t = g_{n,n-1}(\theta_1)a_t g_{n-1,n-2}(\theta_2)\cdots g_{21}(\theta_{n-1}). \tag{49}$$

Since

$$\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & t \end{pmatrix} = \begin{pmatrix} \cos\theta & -t\sin\theta \\ \sin\theta & t\cos\theta \end{pmatrix} = \begin{pmatrix} \lambda' & 0 \\ 0 & \lambda \end{pmatrix}\begin{pmatrix} 1 & x \\ 0 & 1 \end{pmatrix}\begin{pmatrix} \cos\theta' & -\sin\theta' \\ \sin\theta' & \cos\theta' \end{pmatrix}. \tag{50}$$

with

$$\lambda = (\sin^2\theta + t^2\cos^2\theta)^{1/2} = t\left(1 + \frac{1-t^2}{t^2}\sin^2\theta\right)^{1/2}, \tag{51}$$

$$\sin\theta' = \lambda^{-1}\sin\theta, \quad \cos\theta' = \lambda^{-1}t\cos\theta, \tag{52}$$

it follows that

$$\pi_\mu(a_t)f(\theta_1,\theta_2,\ldots\theta_{n-1})$$
$$\left[t\left(1+\frac{1-t^2}{t^2}\sin^2\theta_1\right)^{1/2}\right]^\mu f(\theta_1',\theta_2,\ldots,\theta_{n-1}). \quad (53)$$

Thus the generalized spherical functions [see, for example, Eq. (1.8) of Ref. 20]can be taken as an orthonormal basis for $L_0^2(K)$,

$$Y_{(m_n,m_{n-1},\ldots,m_2)} = N_n \prod_{j=2}^{n-1} C^{m_j+(j-1)/2}_{m_{j+1}-m_j}(\cos\theta_{n-j}) \times \sin^{m_j}\theta_{n-j}\exp(-im_2\theta_{n-1}). \quad (54)$$

In this result the $C_q^p(\cos\theta)$ are Gegenbauer polynomials and N_n is a normalization factor:

$$N_n = (2\pi)^{-1/2}\prod_{j=2}^{n-1}\Gamma\left(m_j+\frac{j-1}{2}\right)2^{m_j+(j-2)/2} \left(\frac{[m_{j+1}+(j-1)/2]\Gamma(m_{j+1}-m_j+1)}{\pi\Gamma(m_{j+1}+m_j+j-1)}\right)^{1/2}. \quad (55)$$

The functions Y are the matrix elements of Eq. (10) for which Σ is a Gel'fand–Zetlin pattern which corresponds to the representations of SO(n) with highest weight $(m_n,0,\ldots,0)$. The number m_k corresponds to the $(n-k+1)$th row of the pattern Σ.

According to Eq. (44) the matrix elements of the operators $\pi_\mu(a_t)$ are given by the integrals

$$(Y_M(\theta_1,\theta_2,\ldots,\theta_{n-1}),\pi_\mu(a_t)Y_{M'}(\theta_1,\theta_2,\ldots,\theta_{n-1})) = \int_{S^{n-1}} d\Omega_n\, Y_M(\theta_1,\theta_2,\ldots,\theta_{n-1}) \left[t\left(1+\frac{1-t^2}{t^2}\sin^2\theta_1\right)^{1/2}\right]^\mu \times Y_{M'}(\theta_1',\theta_2,\ldots\theta_{n-1}). \quad (56)$$

where the integration is over an invariant measure on S^{n-1}, θ_1' is defined by Eq. (52), and M denotes the set of indices $(m_n,m_{n-1},\ldots,m_2)$. The integration in Eq. (56) separates for the variables $\theta_1,\theta_2,\ldots,\theta_{n-1}$. The integration over $\theta_2,\theta_3,\ldots,\theta_{n-1}$ leads to a product of Kronecker deltas $\delta_{m_{n-1},m'_{n-1}}\delta_{m_{n-2},m'_{n-2}}\cdots\delta_{m_2,m'_2}$. Utilizing standard considerations, it can be shown that the matrix element given by Eq. (56) does not depend on $m_{n-2},\ldots,m_2$. Therefore, we denote this matrix element by $d^\mu_{m_n,m'_n,m_{n-1}}(t)$. It is equal to

$$d^\mu_{m_n,m'_n,m_{n-1}}(t) = 2^{2m_{n-1}+n-3}\pi^{-1}\left[\Gamma\left(m_{n-1}+\frac{n-2}{2}\right)\right]^2 \times\left[\left(m_n+\frac{n-2}{2}\right)\left(m'_n+\frac{n-2}{2}\right)\right]^{1/2} \times\left(\frac{(m_n-m_{n-1})!(m'_n-m_{n-1})!}{(m_n+m_{n-1}+n-3)!(m'_n+m_{n-1}+n-3)!}\right)^{1/2} \times\int_0^\pi d\theta_1(\sin^{n-2}\theta_1)(\sin\theta_1)^{m_{n-1}} \times C^{m_{n-1}+(n-2)/2}_{m_n-m_{n-1}}(\cos\theta_1)(\sin\theta_1')^{m_{n-1}} \times C^{m_{n-1}+(n-2)/2}_{m'_n-m_{n-1}}(\cos\theta_1')\left[t\left(1+\frac{1-t^2}{t^2}\sin^2\theta_1\right)^{1/2}\right]^\mu. \quad (57)$$

We denote the expression preceeding the integral sign by N. Then

$$d^\mu_{m_n,m'_n,m_{n-1}}(t) = Nt^{\mu-m_{n-1}}\int_0^\pi d\theta_1(\sin\theta_1)^{2m_{n-1}+n-2} \times\left(1+\frac{1-t^2}{t^2}\sin^2\theta_1\right)^{(\mu-m_{n-1})/2} \times C^{m_{n-1}+(n-2)/2}_{m_n-m_{n-1}}(\cos\theta_1)\{C^{m_{n-1}+(n-2)/2}_{m'_n-m_{n-1}}(\cos\theta_1')\}. \quad (58)$$

For C_p^λ there exists the expansion (Ref. 21)

$$C_p^\lambda(\cos\theta) = \frac{1}{\Gamma(\lambda)}\sum_{m=0}^{[p/2]}\frac{(-1)^m\Gamma(\lambda+p-m)2^{p-2m}}{m!(p-2m)!}\cos^{p-2m}\theta, \quad (59)$$

where the expression $[p/2]$ denotes the integer part of $p/2$. Subsituting this expansion for C_p^λ into Eq. (58), and taking into account the expressions (51) and (52) for $\sin\theta_1'$ and $\cos\theta_1'$, it follows that (to simplify the notation we replace m_n,m'_n,m_{n-1} by m,m',m_1)

$$d^\mu_{m,m',m_1}(t) = \frac{4N}{[\Gamma(m_1+(n-2)/2)]^2}t^{\mu-m_1} \times\sum_{k=0}^{[(m-m_1)/2][(m'-m_1)/2]}\sum_{k'=0}\frac{(-1)^{k+k'}\Gamma(m+(n-2)/2-k)}{k!k'!(m-m_1-2k)!} \times\frac{\Gamma(m'+(n-2)/2-k')2^{m+m'-2(m_1+k+k')}}{(m'-m_1-2k')!} \times\int_0^\pi d\theta(\sin\theta)^{2m_1+n-2}(\cos\theta)^{m+m'-2m_1-2k-2k'} \times\left(1+\frac{1-t^2}{t^2}\sin^2\theta\right)^{(\mu-m'+2k')/2} \quad (60)$$

For the evaluation of the integral we make use of formula 3.681 (1) of Ref. 22. According to this formula one has, for even s

$$\int_0^\pi\frac{(\sin\theta)^r(\cos\theta)^s}{(1+k\sin^2\theta)^\rho}d\theta = B\left(\frac{r+1}{2},\frac{s+1}{2}\right){}_2F_1\left(\rho,\frac{r+1}{2},\frac{r+s+2}{2};-k\right). \quad (61)$$

Thus

$$d^\mu_{m,m',m_1}(t) = t^{\mu-m_1}\sum_{k=0}^{[(m-m_1)/2][(m'-m_1)/2]}\sum_{k'=0}N(k,k') \times B\left(m_1+\frac{n-1}{2},\frac{m+m'+1}{2}-m_1-k-k'\right) \times{}_2F_1\left(\frac{-\mu+m'}{2}-k',m_1+\frac{n-1}{2},\frac{m+m'+n}{2}-k-k';\frac{t^2-1}{t^2}\right), \quad (62)$$

where

$$N(k,k') = \frac{4N(-1)^{k+k'}2^{m+m'-2(m_1+k+k')}}{k!k'!(m-m_1-2k)!(m'-m_1-2k')!} \times\frac{\Gamma(m+(n-2)/2-k)\Gamma(m'+(n-2)/2-k')}{[\Gamma(m_1+(n-2)/2)]^2}. \quad (63)$$

7. MATRIX ELEMENTS FOR THE UNITARY REPRESENTATIONS OF THE GROUPS U(n) IN AN SO(n) BASIS

Equation (62) gives the matrix elements of the operators $\pi_\mu^\pm(a_t)$ for the representations of the most degenerate unitary series (for $\mu = i\tau - n/2, \tau\in R$) of the group GL($n,R$) [and consequently also for SL(n,R)], as well as the matrix elements for the representations $\pi_\mu^\pm$, where μ is an arbitrary complex number. We use these matrix elements to derive the

corresponding matrix elements for the unitary irreducible representations of U(n) in an SO(n) basis. In the following we use the method which was suggested in Ref. 16 (see also Ref. 17).

It was pointed out at the begin of Sec. 6 that the representations $\pi_\mu^\pm$ of GL(n,R) differ from the representations $\pi^\pm{}_\mu$ of SL(n,R), introduced in Sec. 2, by a multiplier only. This multiplier forms a one-dimensional representation of R_0. Therefore, the results which were obtained for SL(n,R) transfer trivially to GL(n,R).

We consider the matrix elements given by Eqs. (62) and (63) for those representations $\pi_\mu^\pm$ that contain finite-dimensional subrepresentations of GL(n,R), i.e., for the representations $\pi_\mu^\pm$ with $\mu = 0,1,2,\cdots$. For the values $m,m' = \mu,\mu-2,\mu-4,\ldots 0$ (or 1) Eqs. (62) and (63) give the matrix elements for finite-dimensional representations of GL(n,R). Analytic continuation of t to $e^{i\vartheta}$, $0 \leqslant \vartheta < 2\pi$, leads to matrix elements for finite-dimensional representations of U(n). The representation matrices which are obtained are, however, not unitary.

In order to obtain unitary representations the basis $|m,\Sigma\rangle$ has to be changed to the basis $|m,\Sigma\rangle'$ by means of the formulas (32)–(35). The matrix elements for the representations of U(n) with highest weight (M,0,...,0) are then given in the new basis by

$$\tilde{d}^{M}_{m,m',m_1}(e^{i\vartheta}) = [\lambda^{\pm}_{m}/\lambda^{\pm}_{m'}]^{1/2} d^{M}_{m,m',m_1}(e^{i\vartheta}), \tag{64}$$

where the $\lambda^{\pm}_{m}$ are defined by Eqs. (33) and (35), with $\sigma = -M$, and the matrix elements $d^{M}_{m,m',m_1}(e^{i\vartheta})$ are defined by Eqs. (62) and (63). If M is even, then the plus sign applies in Eq. (64); if M is odd, then the minus sign is to be taken.

It was mentioned before that in the basis $|m,\Sigma\rangle'$ the representations $\pi_\mu^\pm$ of the principal most degenerate unitary series also leads to unitary matrices. In the basis $|m,\Sigma\rangle'$ the matrix elements for these representations are given by

$$\tilde{d}^{\mu}_{m,m',m_1}(t) = [\lambda^{\pm}_{m}/\lambda^{\pm}_{m'}]^{1/2} d^{\mu}_{m,m',m_1}(t),$$

where the $\lambda^{\pm}_{m}$ are given by Eqs. (33) and (35) with $\mu = -\sigma$.

Formula (64) gives the representation matrix elements for the elements of U(n) which correspond to the subgroup

$$\mathrm{diag}(1,1,\ldots,1,e^{i\vartheta}). \tag{65}$$

These matrix elements, together with the representation matrix elements for the group elements of SO(n), define completely the matrix elements for all the operators of U(n) with respect to an SO(n) basis, in precisely the same way as was the case for the group GL(n,R)

Formula (64) expresses the matrix elements for the representations of U(n) by means of hypergeometric functions. Since now M is an integer, the hypergeometric function reduces to a finite series [in Eq. (62) $(-\mu+m')/2-k \equiv (-M+m')/2-k$ is now a negative integer]. According to 8.962 (1) of Ref. 22 this finite hypergeometric series can be represented by means of Jacobi polynomials.

Finally let us mention that Eq. (62) contains a B function, $B(x,y)$, with nonnegative half-integer arguments. This function can be represented as a ratio of products of factorials. According to 8.335 (1) of Ref. 22 one has

$$\Gamma(p+\tfrac{1}{2}) = (\pi)^{1/2} 2^{2p-1} \Gamma(2p)/\Gamma(p), \tag{66}$$

where p is a nonnegative integer. Thus

$$B(x,y) = \Gamma(x)\Gamma(y)/\Gamma(x+y).$$

Equation (66) can also be utilized in the expression for $N(k,k')$ given by Eq. (63), in which Γ functions with half-integer arguments can appear.

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Second and fourth indices of plethysms [a)]

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(Received 14 April 1981; accepted for publication 22 May 1981)

The direct product of several copies of a representation decomposes into a direct sum of components each with a definite permutation symmetry. The decomposition of any of the components into a direct sum of irreducible representations is the computation of a plethysm. The decomposition is often simply effected when the dimension and its analogs, the second and fourth indices of the plethysm, are known. The paper contains formulas for second and fourth indices of many specific plethysms as well as a prescription for the general plethysm. The same formula is valid for the plethysm based on any finite representation of any semisimple Lie algebra. Applications are illustrated by decomposition of all plethysms of degree 3 based on the E_8 representation of dimension 3875; all fourth-degree E_8-scalars are enumerated.

PACS numbers: 02.20.Qs

I. INTRODUCTION

The second and fourth indices[1] of representations of semisimple Lie groups, together with the dimension, have proven useful in finding branching rules and Clebsch–Gordan series[1,2] and for other, physical, applications.[3] They can be just as useful in the computation of plethysms; a plethysm is the component, whose permutation symmetry is prescribed by a Young tableau, of the direct product of n copies of some representation R. When no ambiguity can arise, we may use the terms plethysm and Young tableau interchangeably.

The $(2n)$ index $I_{\lambda}^{(2n)}$ of a representation (λ) is defined as the sum of the $(2n)$th powers of the magnitudes of the weights of (λ); in particular, $I_{\lambda}^{(0)}$ is the dimension of (λ).

The purpose of this paper is to provide formulas for the second and fourth indices of plethysms of any symmetry. An attractive property of these formulas is that they depend on the representation R only through its dimension and the rank of the group it represents; only one formula is needed for each Young tableau and each index. We are doing for the second and fourth indices what was done recently[4] for the SU (n) triangle anomaly number.

Section II contains explicit expressions for $I^{(2)}$ and $I^{(4)}$ of some Young tableaux. In Sec. III two general relations are established [Eqs. (29) and (30)] and a general derivation of $I^{(2)}$ and $I^{(4)}$ formulas is described. Section IV contains an example of application: determination of all scalars of degree 4 and computation of all three-box plethysms based on the E_8 representation of dimension 3875. Some observations are made in Sec. V

II. RESULTS FOR PARTICULAR YOUNG TABLEAUX

In this section we present formulas for second and fourth indices of plethysms corresponding to some particular Young tableaux. In the following section we explain how they are obtained, and how one could find the analogous formulas for any plethysm.

We denote the representation R on which the plethysm is based by a single box $\square$. The representation R may be reducible or irreducible. Its dimension is $I_{\square}^{(0)} = N$, its second index is $I_{\square}^{(2)}$ and its fourth index is $I_{\square}^{(4)}$. Formulas for $I_{\square}^{(2)}$ and $I_{\square}^{(4)}$ for representations of semisimple groups are given in Ref. 1; numerical tables are found in Ref. 5. A plethysm is denoted by its Young tableau.

For Young tableaux of up to four boxes the formulas are

$$I^{(2)}_{\square\square} = (N+2)I^{(2)}_{\square}, \tag{1}$$

$$I^{(2)}_{\begin{smallmatrix}\square\\\square\end{smallmatrix}} = (N-2)I^{(2)}_{\square}, \tag{2}$$

$$I^{(2)}_{\square\square\square} = \tfrac{1}{2}(N+2)(N+3)I^{(2)}_{\square}, \tag{3}$$

$$I^{(2)}_{\begin{smallmatrix}\square\square\\\square\end{smallmatrix}} = (N^2-3)I^{(2)}_{\square}, \tag{4}$$

$$I^{(2)}_{\begin{smallmatrix}\square\\\square\\\square\end{smallmatrix}} = \tfrac{1}{2}(N-2)(N-3)I^{(2)}_{\square}, \tag{5}$$

$$I^{(2)}_{\square\square\square\square} = \tfrac{1}{6}(N+2)(N+3)(N+4)I^{(2)}_{\square}, \tag{6}$$

$$I^{(2)}_{\begin{smallmatrix}\square\square\square\\\square\end{smallmatrix}} = \tfrac{1}{2}(N+2)(N^2+N-4)I^{(2)}_{\square}, \tag{7}$$

$$I^{(2)}_{\begin{smallmatrix}\square\square\\\square\square\end{smallmatrix}} = \tfrac{1}{3}N(N-2)(N+2)I^{(2)}_{\square}, \tag{8}$$

$$I^{(2)}_{\begin{smallmatrix}\square\square\\\square\\\square\end{smallmatrix}} = \tfrac{1}{2}(N-2)(N^2-N-4)I^{(2)}_{\square}, \tag{9}$$

$$I^{(2)}_{\begin{smallmatrix}\square\\\square\\\square\\\square\end{smallmatrix}} = \tfrac{1}{6}(N-2)(N-3)(N-4)I^{(2)}_{\square}, \tag{10}$$

$$I^{(4)}_{\square\square} = (N+8)I^{(4)}_{\square} + [(l+2)/l\,]I^{(2)2}_{\square}, \tag{11}$$

$$I^{(4)}_{\begin{smallmatrix}\square\\\square\end{smallmatrix}} = (N-8)I^{(4)}_{\square} + [(l+2)/l\,]I^{(2)2}_{\square}, \tag{12}$$

$$I^{(4)}_{\square\square\square} = \tfrac{1}{2}(N^2+17N+54)I^{(4)}_{\square} + (N+4)[(l+2)/l\,]I^{(2)2}_{\square}, \tag{13}$$

[a)]Work supported in part by the Natural Science and Engineering Research Council of Canada and by the Ministére de l'Education du Québec.

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$$I^{(4)}_{\square\square\atop\square\square} = (N^2-27)I^{(4)}_{\square} + 2N\,[(l+2)/l\,]I^{(2)^2}_{\square}, \tag{14}$$

$$I^{(4)}_{\square\atop\square\atop\square\atop\square} = \tfrac{1}{2}(N^2-17N+54)I^{(4)}_{\square} + (N-4)[(l+2)/l\,]I^{(2)^2}_{\square}, \tag{15}$$

$$I^{(4)}_{\square\square\square\square} = \tfrac{1}{6}(N+4)(N^2+23N+96)I^{(4)}_{\square} + \tfrac{1}{2}(N+4)(N+5)[(l+2)/l\,]I^{(2)^2}_{\square}, \tag{16}$$

$$I^{(4)}_{\square\square\atop\square\square\atop\square} = \tfrac{1}{2}(N+8)(N^2+N-16)I^{(4)}_{\square} + \tfrac{1}{2}(3N^2+9N-8)[(l+2)/l\,]I^{(2)^2}_{\square}, \tag{17}$$

$$I^{(4)}_{\square\square\atop\square\square} = \tfrac{1}{3}N(N^2-58)I^{(4)}_{\square} + (N^2+2)[(l+2)/l\,]I^{(2)^2}_{\square}, \tag{18}$$

$$I^{(4)}_{\square\square\atop\square\atop\square} = \tfrac{1}{2}(N-8)(N^2-N-16)I^{(4)}_{\square} + \tfrac{1}{2}(3N^2-9N-8)[(l+2)/l\,]I^{(2)^2}_{\square}, \tag{19}$$

$$I^{(4)}_{\square\atop\square\atop\square\atop\square} = \tfrac{1}{6}(N-4)(N^2-23N+96)I^{(4)}_{\square} + \tfrac{1}{2}(N-4)(N-5)[(l+2)/l\,]I^{(2)^2}_{\square}, \tag{20}$$

Here l is the rank of the group represented by $\square$.

For Young tableaux with one row or one column, or for one row or one column with a single additional box, the second index is

$$I^{(2)}_{\square\square\atop\leftarrow k\rightarrow} = \frac{(N+k)!}{(N+1)!(k-1)!}I^{(2)}_{\square}, \tag{21}$$

$$I^{(2)}_{\square\atop\square\atop k\atop\square\atop\square} = \frac{(N-2)!}{(N-k-1)!(k-1)!}I^{(2)}_{\square}, \tag{22}$$

$$I^{(2)}_{\square\square\atop\square\atop\leftarrow k\rightarrow} = \frac{(N+k-1)!}{(N+1)!(k-1)!}[N^2+N(k-2)-k-1]I^{(2)}_{\square}, \tag{23}$$

$$I^{(2)}_{\square\square\atop\square\atop k\atop\square} = \frac{(N-2)!}{(N-k)!(k-1)!}[N^2-N(k-2)-k-1]I^{(2)}_{\square}. \tag{24}$$

Equating the indices of both sides of the identity

$$\square\otimes\square\otimes\square\otimes\square = \square\square\square\square \oplus 3\,\square\square\square \oplus 2\,\square\square \oplus 3\,\square\atop\square \oplus \square\atop\square\atop\square$$

provides a useful check on our results. The coefficients on the right are the dimensions of the representations of the group S_4 corresponding to the Young tableaux. The left side is known from the general formula for indices of a direct product [Eqs.(15) and (16) of Ref. 1 or Eqs. (2.10) and (2.11) of Ref. 5]. Clearly a similar identity holds for a product of any number of representations $\square$.

III. GENERAL PROPERTIES AND DERIVATIONS

In this section we indicate how the formulas of Sec. II are found and show how to derive a formula for the second and fourth indices of any plethysm.

As a simple illustrative example we first derive (1), (2), (11), and (12), the second and fourth indices of two-box plethysms. The Young tableaux $\square\square$ and $\square\atop\square$ refer to the symmetric and antisymmetric components of the direct product of two copies of the representation denoted by $\square$. Clearly

$$\square\otimes\square = \square\square \oplus \square\atop\square. \tag{25}$$

Also, we may write symbolically

$$\square\square = \square^2 \cup \square\atop\square, \tag{26}$$

where $\square^2$ denotes the weights of $\square$ with the scale doubled. Equation (26) states the obvious fact that the weights of $\square\square$ are just those contained in $\square\atop\square$ together with those of $\square^2$. Similarly (25) has a straightforward interpretation in terms of weights. Since the indices are defined in terms of weights, Eqs. (25) and (26) lead immediately to relations for indices. According to Ref. 1,

$$I^{(2)}_{\square\otimes\square} = 2NI^{(2)}_{\square} \tag{27}$$

and

$$I^{(4)}_{\square\otimes\square} = 2NI^{(4)}_{\square} + [2(l+2)/l\,]I^{(2)^2}_{\square}. \tag{28}$$

Obviously, $I^{(2)}_{\square^2} = 4I^{(2)}_{\square}$ and $I^{(4)}_{\square^2} = 16I^{(4)}_{\square}$. Equations (1), (2), (11), and (12) follow.

We now wish to demonstrate the general relations

$$I^{(2)}_{\mathrm{YT}} = P_{\mathrm{YT}}(N)I^{(2)}_{\square}, \tag{29}$$

$$I^{(4)}_{\mathrm{YT}} = Q_{\mathrm{YT}}(N)I^{(4)}_{\square} + [(l+2)/l\,]R_{\mathrm{YT}}(N)I^{(2)^2}_{\square}, \tag{30}$$

where YT is an arbitrary Young tableau of p boxes. N is the dimension of the representation $\square$ and l is the rank of the group. $P_{\mathrm{YT}}(N)$, $Q_{\mathrm{YT}}(N)$, and $R_{\mathrm{YT}}(N)$ are polynomials in N of degrees $p-1$, $p-1$, and $p-2$ respectively; they do not depend on the group or on $\square$ except through the dimension N.

The proof of (29) coincides with the proof of Eq. (3.1) of Ref. 4, and is not repeated here. The proof of (30) is also very similar. The difference is that the formula

$$I^{(4)}_{(\lambda_1)\otimes\cdots\otimes(\lambda_k)} = \left(\prod_{j=1}^{k}N_j\right)\sum_{i=1}^{k}\frac{I^{(4)}_{\lambda_i}}{N_{\lambda_i}} + \left(\prod_{n=1}^{k}N_{\lambda_n}\right)\sum_{i>j=1}^{k}\frac{I^{(2)}_{\lambda_i}I^{(2)}_{\lambda_j}}{N_{\lambda_i}N_{\lambda_j}} \tag{31}$$

for the fourth index of the direct product of k representations $(\lambda_1),\ldots,(\lambda_k)$ replaces formula (A5), Ref. 4.

The polynomials $P_{\mathrm{YT}}(N)$ for conjugate Young tableaux (obtained from each other by transposition) are simply related. One is obtained from the other by changing the sign of terms whose degree in N differs by an odd integer from the degree of the polynomial. The same statement holds for $Q_{\mathrm{YT}}(N)$ and $R_{\mathrm{YT}}(N)$. The proof follows from the expressions for Young tableaux in terms of symmetric polynomials.[6]

A pedestrian, but practical, derivation of $I^{(2)}_{\mathrm{YT}}$ (or $I^{(4)}_{\mathrm{YT}}$) for a Young tableau of p boxes starts with Eq. (29) [or (30)]. Since $P_{\mathrm{YT}}(N)$ contains p [$Q_{\mathrm{YT}}(N)$ and $R_{\mathrm{YT}}(N)$ together contain $2p-1$] undetermined coefficients, it suffices to choose p (or $2p-1$) representations of the same or different groups with different N. Each N must be at least as great as the number of rows in YT. Substitution of the values of N, $I^{(2)}_{\square}$, $I^{(2)}_{\mathrm{YT}}$ [or N, $I^{(2)}_{\square}$, $I^{(4)}_{\square}$, $I^{(4)}_{\mathrm{YT}}$] yields linear equations

which determine the unknown coefficients. The values of the plethysms YT, given by branching rules for SU(N) to the group in question, are provided by the tables of Ref. 5.

The derivation of Eq. (22) begins with the identity

$$[1^k] = k^{-1} \sum_{j=1}^{k} (-1)^{j-1} [1^{k-j}] \otimes \square^j, \tag{32}$$

where $[1^k]$ stands for the weights of the plethysm whose Young tableau consists of a single column of length k, and $\square^j$ stands for the weights of $\square$ with scale increased by a factor j. The proof of (22) proceeds by induction. Take the second index of both sides of (32), using Eq. (15) of Ref. 1 to evaluate the index of the direct product, and assuming the validity of (22) for $j < k$. The result is

$$I^{(2)}_{[1^k]} = k^{-1} I^{(2)}_{\square} \sum_{j=1}^{k} (-1)^{j-1} \times \left(\frac{N(N-2)!}{(N-k+j-1)!(k-j-1)!} + \frac{j^2 N!}{(N-k+j)!(k-j)!} \right). \tag{33}$$

The sum on the right side of (33) may be evaluated by noticing that it is a polynomial in N of degree $k-1$ whose leading term is $kN^{k-1}/(k-1)!$ and which vanishes for $N = 2,3,...,k$. It is therefore $k(N-2)!/(k-1)!(N-k-1)!$ and (22) is established.

Since the plethysm in (21) is conjugate to that in (22), the right side of (21) is obtained from that of (22) by changing the sign of alternate powers of N. Eq. (24) is obtained from the relation $[1^k] \otimes \square = [1^{k+1}] \oplus [2,1^{k-1}]$, where $[2,1^{k-1}]$ is the Young tableau of (24).

We complete this section by describing a procedure for deriving $I^{(2)}_{\rm YT}$ and $I^{(4)}_{\rm YT}$ for any Young tableau. For completeness we also give $N_{\rm YT}(N) \equiv I^{(0)}_{\rm YT}(N)$, the dimension of the plethysm YT. It is just the dimension of the representation $(\lambda_1,...,\lambda_{N-1})$ of SU(N), where λ_k is the number of columns of length k in YT:

$$N_{\rm YT} = \prod_{i<j}^{N} (l_i - l_j)/(l^0_i - l^0_j), \tag{34}$$

where

$$l_j = \sum_{k=j}^{N-1} \lambda_k + N - j, \quad 1 \leqslant j \leqslant N-1, \qquad l_N = 0, \quad l^0_i = N - i, \quad 1 \leqslant i \leqslant N. \tag{35}$$

Proceeding as in the case of Eq. (29), one verifies that $N_{\rm YT} = L_{\rm YT}(N) \cdot N$, where $L_{\rm YT}$ is a polynomial of degree $p-1$ and N is the dimension of $\square$.

In order to find $I^{(2)}_{\rm YT}$, it suffices to know it for one representation for each value of N. But $I^{(2)}_{\rm YT}$ is known when we take for $\square$ the defining N-dimensional representation of SU(N). It is given[1] by

$$I^{(2)}_{\rm YT} = N_{\rm YT} [N(N+1)]^{-1} \sum_{i<j}^{N} [(l_i - l_j)^2 - (l^0_i - l^0_j)^2]. \tag{36}$$

Since $I^{(4)}_{\rm YT}$ in (30) contains two polynomials $Q_{\rm YT}(N)$ and $R_{\rm YT}(N)$, it suffices to know $I^{(4)}_{\rm YT}$ for two representations, each of dimension N, but with different values of the ratio $(l+2) I^{(2)2}_{\square} [I I^{(4)}_{\square}]^{-1}$. We may take for $\square$ (i) the defining representation of SU(N) and (ii) the direct sum of the defining and scalar representations of SU($N-1$). The left sides of (30) for the two cases are obtained from the formula[1] for $I^{(4)}_{\lambda}$ of an SU(N) irreducible representation $(\lambda) \equiv (\lambda_1,..,\lambda_{N-1})$,

$$I^{(4)}_{\lambda} = F(l) - F(l^0), \tag{37}$$

where

$$F(l) = N_\lambda \Big(p_4(l) \frac{(N-1)(N^2+7N+6)}{N^2(N+1)(N+2)(N+3)} + [p_4(l) - p_1(l) p_3(l)] \frac{N^2+7N-6}{N^2(N+1)(N+2)} + \{3[p_2(l)]^2 - 3[p_1(l)]^2 p_2(l) + [p_1(l)]^4 - p_4(l)\} \frac{1}{N^2} + \{[p_2(l)]^2 + p_1(l) p_3(l) - p_4(l) - [p_1(l)]^2 p_2(l)\} \frac{N-3}{N^2(N+1)} - \tfrac{1}{6} \sum_{i<j}^{N} (l_i - l_j)^2 \Big). \tag{38}$$

Here $p_\alpha(l)$ in (38) is the symmetric function of degree α defined by[7]

$$\prod_{i=1}^{N} (1 - z l_i)^{-1} = \sum_{\alpha} p_\alpha(l) z^\alpha. \tag{39}$$

For case (i), $\square$ the defining representation of SU(N), the left side of (30) is given by Eq. (37), with λ_i equal to the number of columns of YT with length i. On the right side of (30), we put $l = N-1$, $I^{(4)}_{\square} = (N-1)^2/N$, and $I^{(2)}_{\square} = N-1$.

For case (ii), $\square$ the direct sum of the defining and scalar representations of SU($N-1$), the plethysm YT is a direct sum of the SU($N-1$) [not U($N-1$)] representations contained in the reduction of the SU(N) representation (λ) of the preceding paragraph. Their fourth indices are obtained from (37). On the right side of (30), put $l = N-2$, $I^{(4)}_{\square} = (N-2)^2/(N-1)$, and $I^{(2)}_{\square} = N-2$.

To illustrate the method, let us take YT =  , and rederive Eq. (18). For case (i), Eq. (30) reads

$$\tfrac{2}{3}(N-1)(N-2)(2N^2+5N-16) = Q_{\square\!\square}(N) \frac{(N-1)^2}{N} + \frac{N+1}{N-1} R_{\square\!\square}(N)(N-1)^2. \tag{40}$$

For case (ii)  contains the irreducible representations (0 2 0...0), (1 1 0...0), and (2 0...0) of SU($N-1$). Then Eq. (30) reads

$$\frac{N(N-2)}{3(N-1)}(4N^3-5N^2-52N+110)=Q_{\square\square}(N)\frac{(N-2)^2}{N-1}+\frac{N}{N-2}R_{\square\square}(N)(N-2)^2. \tag{41}$$

Solving (40) and (41) for $Q_{\square\square}(N)$ and $R_{\square\square}(N)$, we find the polynomials in Eq. (18).

IV. AN EXAMPLE FROM E_8

As a nontrivial application of the results of Sec. II, we construct all plethysms of two and three boxes based on the 3875-dimensional representation (0 0 0 0 0 0 1 0) of E_8. It turns out that with no further work we can enumerate E_8 scalars in all four-box plethysms; this has some physical interest, for construction of a Higgs potential in a certain unified field theory[8] requires a knowledge of fourth-degree symmetric scalars in the representation (0 0 0 0 0 0 1 0).

Since the index $I^{(2k)}$, $k=0,1,2,\cdots$, of a reducible representation is equal to the sum of the $(2k)$th indices of the irreducible components[1] our procedure is to search, with the help of a computer, for that combination of irreducible representations whose dimensions, and second and fourth indices, add to the required values. To simplify our tabulation, we refer to the irreducible representations of E_8 as 1,2,3,··· in order of increasing dimension. The trivial (scalar) representation is labelled 1, the one of dimension 248 is 2, that of dimension 3875 is 3, etc. In case of equal dimensions (e.g., 32, 33) they are ordered according to increasing second index. For explicit values see p. 79 of Ref. 5.

TABLE I. Multiplicities of irreducible E_8-representations in low plethysms based on the representation □ of dimension 3875. The representations are numbered in order of increasing dimensions and $I^{(2)}$ in case of equal dimensions.

	Plethysm				
Representation	$\square\square$	$\begin{smallmatrix}\square\\\square\end{smallmatrix}$	$\square\square\square$	$\begin{smallmatrix}\square\square\\\square\end{smallmatrix}$	$\begin{smallmatrix}\square\\\square\\\square\end{smallmatrix}$
1	1		1		
2		1		2	1
3	1		3	3	1
4	1		2	2	
5		1	1	3	3
6	1		1	4	1
7		1	2	5	3
8					1
9	1		3	3	1
10			1	3	1
11	1		2	2	
12		1	1	3	2
13			2	3	2
14			1	2	
15			1	3	2
17			1	2	
18			1		
20			1	2	1
21				1	1
22				1	1
23			1	1	1
25				1	
27			1		
30			1	1	
31					1
33				1	

The relevant plethysms are given in Table I. Each column represents a direct sum of representations contained in the corresponding plethysm. By adding the multiplicities in the first two columns, one gets the multiplicities of representations in the direct product $3\otimes 3$. Similarly, the direct product $3\otimes 3\otimes 3$ is given by the sum of columns 3, 5, plus twice column 4. Relevant dimensions and indices of low plethysms are given in Table II.

From the information in Table I we can deduce the number of scalars in each of the five four-box plethysms. Denote by S_{YT} the number of scalars in the plethysm YT. Since the plethysms $\square\square$ and $\begin{smallmatrix}\square\\\square\end{smallmatrix}$ have no irreducible representations in common, the direct product $\square\square\otimes\begin{smallmatrix}\square\\\square\end{smallmatrix}$ contains no scalars. But $\square\square\otimes\begin{smallmatrix}\square\\\square\end{smallmatrix}=\begin{smallmatrix}\square\square\square\\\square\end{smallmatrix}\oplus\begin{smallmatrix}\square\square\\\square\square\end{smallmatrix}$ Hence $S_{\square\square\square\square}=S_{\begin{smallmatrix}\square\square\\\square\square\end{smallmatrix}}=0$. Since $\square\square\square$ contains three copies of the representation 3, it follows that $\square\square\square\otimes\square$ contains three scalars. But $\square\square\square\otimes\square=\square\square\square\square\oplus\begin{smallmatrix}\square\square\square\\\square\end{smallmatrix}$ Hence $S_{\square\square\square\square}=3$. Since $\begin{smallmatrix}\square\\\square\\\square\end{smallmatrix}$ contains one copy of 3, it follows that $\begin{smallmatrix}\square\\\square\\\square\end{smallmatrix}\otimes\square$ contains one scalar. But $\begin{smallmatrix}\square\\\square\\\square\end{smallmatrix}\otimes\square=\begin{smallmatrix}\square\\\square\\\square\\\square\end{smallmatrix}\oplus\begin{smallmatrix}\square\square\\\square\square\end{smallmatrix}$. Hence $S_{\begin{smallmatrix}\square\\\square\\\square\\\square\end{smallmatrix}}=1$. Since $\begin{smallmatrix}\square\square\\\square\square\end{smallmatrix}$ contains three copies of 3, it follows that $\begin{smallmatrix}\square\square\\\square\square\end{smallmatrix}\otimes\square$ contains three scalars. But $\begin{smallmatrix}\square\square\\\square\square\end{smallmatrix}\otimes\square=\begin{smallmatrix}\square\square\square\square\\\square\square\end{smallmatrix}\oplus\begin{smallmatrix}\square\square\square\\\square\square\square\end{smallmatrix}\oplus\begin{smallmatrix}\square\square\square\\\square\square\end{smallmatrix}$. Hence $S_{\begin{smallmatrix}\square\square\square\\\square\square\square\end{smallmatrix}}=3$.

V. COMMENTS

The main advantage of computing plethysms in the way described in the article is in the fact that it is independent of the rank or type of the Lie algebra (group) involved. Once the dimensions and indices for a plethysm are known, the computation is reduced to the same search in a list of dimensions and indices of irreducible representations. The example of Sec. IV was chosen to illustrate the method because it is the largest one we know with physical motivation.[8]

TABLE II. Dimensions, second and fourth indices of the plethysms of the example (Sec. IV) and of Table I. The numbers 31,480, and 960 dividing the dimension, $I^{(2)}$ and $I^{(4)}$, respectively were chosen for convenience [cf. property (42)].

	Dimension/31	$I^{(2)}/480$	$I^{(4)}/960$
□	125	25	43
$\square\square$	242 250	96 925	354 469
$\begin{smallmatrix}\square\\\square\end{smallmatrix}$	242 125	96 825	353 781
$\square\square\square$	313 067 750	187 937 575	1 051 565 911
$\begin{smallmatrix}\square\square\\\square\end{smallmatrix}$	625 651 000	375 390 550	2 098 795 714
$\begin{smallmatrix}\square\\\square\\\square\end{smallmatrix}$	312 583 375	187 453 200	1 047 233 286

In our particular cases, the search yielded unique solutions to our problems. However, it is conceivable that the equalities of dimensions, second, and fourth indices allow several solutions. It appears that such an ambiguity would occur in cases far more complicated than anything of practical interest at present or in the foreseeable future.

During the course of solving the problem of Sec. IV we noticed that the irreducible representations of E_8 fall into three classes characterized by their dimension N (mod 31). Turning then to other simple Lie algebras of rank $\leqslant 8$ we found that all but D_5, D_8, C_7, B_4, B_7, and A_8 have the following property:

$$N = 0, \ +1, \text{ or } -1 \pmod{K}, \tag{42}$$

where K is given by

algebra	A_3	A_4	A_5	A_6	A_7	A_8	B_2	B_3	B_4	B_5	B_6	B_7	B_8
K	5	5	7	7	7	—	5	7	—	11	13	—	17

algebra	C_3	C_4	C_5	C_6	C_7	C_8	D_4	D_5	D_6	D_7	D_8	G_2	F_4	E_6	E_7	E_8
K	7	7	11	13	—	17	7	—	11	7	—	7	13	13	19	31

Obviously (42) is trivial for A_1 and A_2. Analyzing the relatively simple dimension formula for G_2, one finds more specifically, that

$$N = 1 \pmod 7 \quad \text{for representations } (i,i), \quad 0 \leqslant i \leqslant 5$$

$$N = -1 \pmod 7 \quad \text{for representations } (i, 2+3i), \quad 0 \leqslant i \leqslant 5.$$

Here the representation labels are given (mod 7) and in the conventions of Ref. 5.

$N = 0 \pmod 7$ for all other irreducible representations of G_2.

Let us point out that a proof of this observation when K is a prime would follow from the existence of an element of finite order K (in the appropriate Lie group) whose character on irreducible representations takes the values $0, 1, -1$ only. The existence of an element of order 1 + Coxeter number has been proved by Chang[9] for all simple Chevalley groups over the integers; however, the character values have not been established.

The formulas for indices of plethysms found in previous sections remain valid not only if the representation denoted by $\square$ is a direct sum of representations but also if it is a formal difference. It was noticed recently[10] that such differences of representations have some interesting properties. Corresponding plethysms then contain representations with negative multiplicities.

Indices of degree 6 and 8 are also of interest.[1] Formulas for indices $I^{(6)}$ and $I^{(8)}$ of plethysms may be derived. Their applicability is restricted to representations of certain algebras only.[1] Namely, $I^{(6)}$ may be used for plethysms of all simple Lie algebras except A_n $(n > 1)$; the index $I^{(8)}$ of plethysms may be used only for A_1, G_2, F_4, E_6, E_7, and E_8.

Our computation for decomposing plethysms of E_8 used the programming language ALGEB of David Ford with arbitrary length integer facilities on the PDP/11.

ACKNOWLEDGMENT

We are grateful to Dr. I. Bars for interesting discussions of the example involving the group E_8.

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Irreducible representations of the central extension of $Sl(2) \wedge T_2$

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(Received 24 June 1980; accepted for publication 3 October 1980)

Using shift operator techniques a classification is given of the irreducible star representations of the central extension algebra $C(Sl(2) \wedge T_2)$. It is found to possess two generic series of such representations, together with an isolated representation which is just the metaplectic representation of Sl(2). This is the only representation it possesses in common with the superalgebra Osp(2, 1).

PACS numbers: 02.20.Rt, 02.20.Sv, 02.10.Sp

1. INTRODUCTION

In a previous paper[1] a classification was given of the irreducible star representations of the superalgebra Osp(2,1), where the even part satisfied the star (Hermiticity) requirements of the noncompact Sl(2) [or Su(1,1)] algebra. All the IR's were found to be dispin, i.e., subduce to precisely two IR's of SL(2), where the two l values [$l(l+1)$ being the eigenvalue of the Sl(2) invariant L^2] differ by $\frac{1}{2}$. One of these representations, corresponding to the l values $-\frac{3}{4}$ and $-\frac{1}{4}$, was seen to be a simple example of a metaplectic representation, considered in greater generality by Sternberg and Wolf.[2]

Here we consider another algebra (in this case a Lie algebra) which also possesses the same metaplectic representation among its irreducible representations. This algebra is the central extension of the semidirect product algebra $Sl(2) \wedge T_2$. We shall give a classification of the irreducible star representations of both algebras; it turns out, in fact, that $Sl(2) \wedge T_2$ possesses only projective star IR's.

A basis for both $Sl(2) \wedge T_2$ and $C(Sl(2) \wedge T_2)$ consists of the Sl(2) basis $\{l_0, l_\pm\}$ and the T_2 basis $\{p_{\pm\frac{1}{2}}\}$ which satisfy the commutation relations

$$[l_0, l_\pm] = \pm l_\pm, [l_+, l_-] = 2l_0,$$
$$[l_0, p_{\pm\frac{1}{2}}] = \pm\tfrac{1}{2} p_{\pm\frac{1}{2}}, \quad [l_\pm, p_{\mp\frac{1}{2}}] = p_{\pm\frac{1}{2}},$$
$$[p_{\frac{1}{2}}, p_{-\frac{1}{2}}] = \gamma I, \tag{1.1}$$

where I is the identity operator and $\gamma = 0$ for $Sl(2) \wedge T_2$. For $C(Sl(2) \wedge T_2)$, γ is an arbitrary nonzero number which, without loss of generality, can be chosen to be $\gamma = i$; the reason we make this choice rather than the obvious $\gamma = 1$ is for convenience of comparison of the metaplectic representation for this algebra and for Osp(2,1).

The algebras have one independent Sl(2) scalar operator

$$Y_+ = -(p_{\frac{1}{2}} p_{-\frac{1}{2}} l_0 + p_{-\frac{1}{2}} p_{\frac{1}{2}} l_0 + p^2_{-\frac{1}{2}} l_+ - p^2_{\frac{1}{2}} l_-) \tag{1.2}$$

and a single invariant

$$I_3 = 2\gamma L^2 - Y_+; \tag{1.3}$$

for $Sl(2) \wedge T_2$, Y_+ is itself an invariant operator. Let R be the operator with eigenvalue l, so $R(R+1) = L^2$; then the following operators, which shift l and the eigenvalue m of l_0 by $\pm\frac{1}{2}$, will be used to classify the IR's of the algebras[3]:

$$O^{\frac{1}{2},\frac{1}{2}} = p_{\frac{1}{2}}(l_0 + R + 1) + p_{-\frac{1}{2}} l_+, \tag{1.4}$$
$$O^{-\frac{1}{2},-\frac{1}{2}} = -p_{-\frac{1}{2}}(l_0 + R) + p_{\frac{1}{2}} l_-. \tag{1.5}$$

Throughout this paper we shall be considering IR's for which the Sl(2) subalgebra satisfies the star conditions $l_0^\dagger = l_0, l_\pm^\dagger = -l_\mp$. Had we taken $l_\pm^\dagger = l_\mp$, i.e., the star conditions appropriate to a compact SU(2) algebra, then, as is well known, it would not be possible to close the $\{p_{\pm\frac{1}{2}}\}$ with respect to the star operation. However it is easy to check that with the Sl(2) star conditions, one may have $p^\dagger_{\pm\frac{1}{2}} = b p_{\mp\frac{1}{2}}$ provided, for $Sl(2) \wedge T_2$, only that $|b|^2 = 1$. For $C(Sl(2) \wedge T_2)$ one also needs $b^2 = \gamma^*/\gamma$. Thus whether $\gamma = 0$ or $\gamma = i$ one may take $b = i$, so we look for IR's of both algebras satisfying the star conditions $l_0^\dagger = l_0$, $l_\pm^\dagger = -l_\mp$, and $p^\dagger_{\pm\frac{1}{2}} = i p_{\mp\frac{1}{2}}$.

As a consequence of this, $(L^2)^\dagger = L^2$ but $Y^\dagger_+ = -Y_+$ and $I_3^\dagger = -I_3$. Also, using standard techniques,[1,3] one can easily show that

$$(O^{1/2,1/2})^\dagger(2R+1) = -iO^{-\frac{1}{2},-\frac{1}{2}}(2R),$$
$$(O^{-\frac{1}{2},-\frac{1}{2}})^\dagger(2R+1) = -iO^{1/2,1/2}(2R+2). \tag{1.6}$$

Thus, when acting on eigenstates $|k; l,m\rangle$ of L^2 and l_0, one obtains the relations

$$\langle k; l \pm \tfrac{1}{2}, m \pm \tfrac{1}{2} | O^{\pm\frac{1}{2},\pm\frac{1}{2}}_{l,m} | k; l, m\rangle = i(2l+1)/(2l+1\pm 1)\langle k; l \pm \tfrac{1}{2}, m \pm \tfrac{1}{2} | (O^{\mp\frac{1}{2},\mp\frac{1}{2}}_{l\pm\frac{1}{2},m\pm\frac{1}{2}})^\dagger | k; l, m\rangle, \tag{1.7}$$

and

$$\langle k; l, m | O^{\mp\frac{1}{2},\mp\frac{1}{2}}_{l\pm\frac{1}{2},m\pm\frac{1}{2}} O^{\pm\frac{1}{2},\pm\frac{1}{2}}_{l,m} | k; l, m\rangle = i(2l+1\pm 1)/(2l+1) |\langle k, l \pm \tfrac{1}{2}, m \pm \tfrac{1}{2} | O^{\pm\frac{1}{2},\pm\frac{1}{2}}_{l,m} | k; l, m\rangle|^2. \tag{1.8}$$

In the above two relations, k is an extra state-labeling parameter. As we shall see, no l degeneracies occur, and k can be defined in terms of the eigenvalue of the invariant of the algebra.

2. IRREDUCIBLE REPRESENTATIONS of $Sl(2) \wedge T_2$

For $Sl(2) \wedge T_2$, $\gamma = 0$, i.e., $p_{\pm\frac{1}{2}}$ mutually commute. In this case $I_3 = -Y_+$, so that Y_+ is itself the invariant of the

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algebra. One may easily check that, when acting on eigenstates of L^2 and l_0,

$$O^{\frac{1}{2},\frac{1}{2}}_{l+\frac{1}{2},m+\frac{1}{2}} O^{\frac{1}{2},\frac{1}{2}}_{l,m} = (l+m+1)Y_+, \tag{2.1}$$

$$O^{\frac{1}{2},\frac{1}{2}}_{l-\frac{1}{2},m-\frac{1}{2}} O^{-\frac{1}{2},-\frac{1}{2}}_{l,m} = (l+m)Y_+. \tag{2.2}$$

Suppose that, within an I.R., l has a minimum value $\underline{l}$, i.e., $O^{-\frac{1}{2},-\frac{1}{2}}_{\underline{l},m}|k;L,m\rangle = 0$ for all values of m within the corresponding I.R. of Sl(2). Thus also $O^{\frac{1}{2},\frac{1}{2}}_{L-\frac{1}{2},m-\frac{1}{2}} O^{-\frac{1}{2},-\frac{1}{2}}_{L,m}|k;L,m\rangle = 0$ so, by Eq. (2.2), since $(\underline{l}+m+1)$ cannot vanish for all m values, $Y_+ = 0$. Hence by Eq. (2.1), $O^{-\frac{1}{2},-\frac{1}{2}}_{L+\frac{1}{2},m+\frac{1}{2}} O^{\frac{1}{2},\frac{1}{2}}_{L,m}|k;L,m\rangle = 0$ which, using Eq. (1.8), implies that $O^{\frac{1}{2},\frac{1}{2}}_{L,m}|k;L,m\rangle = 0$ and L is therefore also the maximum l-value for the I.R. and so the only l-value within the I.R. Furthermore, since the matrix elements of the $p_{\pm\frac{1}{2}}$ are proportional to those of $O^{\pm\frac{1}{2},\pm\frac{1}{2}}$, $p_{\pm\frac{1}{2}}$ themselves vanish for all states of the I.R. Thus such an I.R. of $\mathrm{Sl}(2)\wedge T_2$ reduces to just a single I.R. of Sl(2) and contains no further structure. Clearly an analogous argument holds if the I.R. possesses a maximum l-value, so an I.R. of $\mathrm{Sl}(2)\wedge T_2$ containing more structure than that due to Sl(2) alone can possess no maximum or minimum l-value, and must correspond to a nonzero value of Y_+.

Let $Y_+|k;l,m\rangle = ik|k;l,m\rangle$, where k is real and nonzero. Then substituting from Eqs. (2.1) and (2.2) into Eq. (1.8), we obtain

$$|\langle k;l+\tfrac{1}{2},m+\tfrac{1}{2}|O^{\frac{1}{2},\frac{1}{2}}_{l,m}|k;l,m\rangle|^2 = k(2l+1)(l+m+1)(2l+2)^{-1}, \tag{2.3}$$

and

$$|\langle k;l-\tfrac{1}{2},m-\tfrac{1}{2}|O^{-\frac{1}{2},-\frac{1}{2}}_{l,m}|k;l,m\rangle|^2 = k(2l+1)(l+m)(2l+1)^{-1}. \tag{2.4}$$

Suppose first that $k>0$; then Eqs. (2.3) and (2.4) show that for a star I.R. of $\mathrm{Sl}(2)\wedge T_2$ we must have, for all l and m values within the I.R., $(l+1)^{-1}(2l+1)(l+m+1)\geqslant 0$ and $l^{-1}(2l+1)(l+m)\geqslant 0$. Now if $-1<l<-\frac{1}{2}$, the inequalities require both $(l+m+1)\leqslant 0$ and $(l+m)\geqslant 0$, which is clearly impossible; but since l has no maximum or minimum values and therefore takes on an infinity of values differing by integral multiples of $\frac{1}{2}$, within an I.R. there must be one value of l satisfying $-1<l<-\frac{1}{2}$, and hence violating the star conditions, unless the range of l actually consists precisely of 0, $\pm\frac{1}{2}$, ± 1, $\pm\frac{3}{2}$,.... In this case, however, the range of l includes the values 0 and -1, for which the matrix elements of $O^{\pm\frac{1}{2},\pm\frac{1}{2}}$, and therefore of the $p_{\pm\frac{1}{2}}$ themselves, become singular.

Had we chosen $k<0$, we should find that an l-value between $-\frac{1}{2}$ and 0 would violate the star conditions. Hence we conclude that $\mathrm{Sl}(2)\wedge T_2$ possesses no star I.R.'s apart from those for which the $p_{\pm\frac{1}{2}}$ are identically zero.

3. IRREDUCIBLE REPRESENTATIONS OF $C(\mathrm{Sl}(2)\wedge T_2)$

For $C(\mathrm{Sl}(2)\wedge T_2)$ we choose $\gamma = i$. In this case, therefore, the invariant is $I_3 = 2iL^2 - Y_+$, and the states of the I.R.'s may be labelled by the eigenvalues of I_3. We define the label n by

$$I_3|n;l,m\rangle = in(2n+1)|n;l,m\rangle. \tag{3.1}$$

The eigenvalue of Y_+ is then determined in terms of n and l, so we need consider Y_+ no further.

The shift operators now satisfy

$$O^{-\frac{1}{2},-\frac{1}{2}}_{l+\frac{1}{2},m+\frac{1}{2}} O^{\frac{1}{2},\frac{1}{2}}_{l,m} = (l+m+1)(Y_+ + i(l+1)I), \tag{3.2}$$

$$O^{\frac{1}{2},\frac{1}{2}}_{l-\frac{1}{2},m-\frac{1}{2}} O^{-\frac{1}{2},-\frac{1}{2}}_{l,m} = (l+m)(Y_+ - ilI). \tag{3.3}$$

Using Eq. (3.1) we therefore have

$$O^{-\frac{1}{2},-\frac{1}{2}}_{l+\frac{1}{2},m+\frac{1}{2}} O^{\frac{1}{2},\frac{1}{2}}_{l,m}|n;l,m\rangle = i(l+m+1)(l+n+1)(2l-2n+1)|n;l,m\rangle, \tag{3.4}$$

$$O^{\frac{1}{2},\frac{1}{2}}_{l-\frac{1}{2},m-\frac{1}{2}} O^{-\frac{1}{2},-\frac{1}{2}}_{l,m}|n;l,m\rangle = i(l+m)(l-n)(2l+2n+1)|n;l,m\rangle. \tag{3.5}$$

Comparison of these equations with Eq. (1.8) then yields

$$|\langle l+\tfrac{1}{2},m+\tfrac{1}{2}|O^{\frac{1}{2},\frac{1}{2}}_{l,m}|l,m\rangle|^2 = (l+m+1)(l+n+1)(2l-2n+1)\times(2l+1)(2l+2)^{-1}. \tag{3.6}$$

and

$$|\langle l-\tfrac{1}{2},m-\tfrac{1}{2}|O^{-\frac{1}{2},-\frac{1}{2}}_{l,m}|l,m\rangle|^2 = (l+m)(l-n)(2l+2n+1)(2l+1)(2l)^{-1} \tag{3.7}$$

which give the star conditions to be satisfied by the I.R.'s, namely that for all states of the I.R., $(l+m+1)(l+n+1)(2l-2n+1)(2l+1)(l+1)^{-1}$ and $(l+m)(l-n)(2l+2n+1)(2l+1)(l)^{-1}$ must be real and non-negative. Furthermore we see from Eqs. (3.4) and (3.5) that any minimum or maximum l-values occuring for the I.R. of $C(\mathrm{Sl}(2)\wedge T_2)$ corresponding to $I_3 = in(2n+1)$ must satisfy $l=n$ or $-(n+\frac{1}{2})$ and $\bar{l} = -(n+1)$ or $(n-\frac{1}{2})$. Also, since the I.R. are labelled by $n(2n+1)$, which is symmetric about $n=-\frac{1}{4}$, rather than by n itself, we may impose without loss of generality the restriction $n\geqslant -\frac{1}{4}$ for real n.

The I.R.'s of Sl(2) are well known[5] and summarized in the previous paper by the author.[1] The principal series of representations cannot occur since $O^{\pm\frac{1}{2},\pm\frac{1}{2}}$ acting on a state for which $l=-\frac{1}{2}+i\rho$ with ρ real would produce states with $l=i\rho$ or $-1+i\rho$, which would violate the internal Sl(2) star conditions. This means that only the supplementary or discrete Sl(2) representations can arise, for all of which l is real.

First we consider the possibility that n be complex. The reality of $n(2n+1)$ shows that the only possibility is $n=-\frac{1}{4}+ib$ where b is real and nonzero. The star conditions (3.6) and (3.7) then become

$$(l+m+1)(2l^2+3l+2b^2+\tfrac{9}{8})(2l+1)(l+1)^{-1}\geqslant 0$$

and

$$(l+m)(2l^2+l+2b^2+\tfrac{1}{8})(2l+1)l^{-1}\geqslant 0.$$

Since l is real and $b\neq 0$, $(2l^2+3l+2b^2+\frac{9}{8})$ and $(2l^2+l+2b^2+\frac{1}{8})$ are always positive and nonzero, so l can have no maximum or minimum value. Hence, unless l is half-integral, there must be an l-value inbetween -1 and $-\frac{1}{2}$, where the star conditions require the impossible $l+m+1\leqslant 0$ and $l+m\geqslant 0$. If l is half-integral, then $l=0$ and $l=-1$, where the matrix elements of the $O^{\pm\frac{1}{2},\pm\frac{1}{2}}$ become singular, would occur. We therefore conclude that no star I.R.'s for which n is complex can exist.

Now we consider what star I.R.'s occur for real n. In addition to the positivity conditions for the l-shifting operators, we also have the internal Sl(2) star conditions that l_+l_-

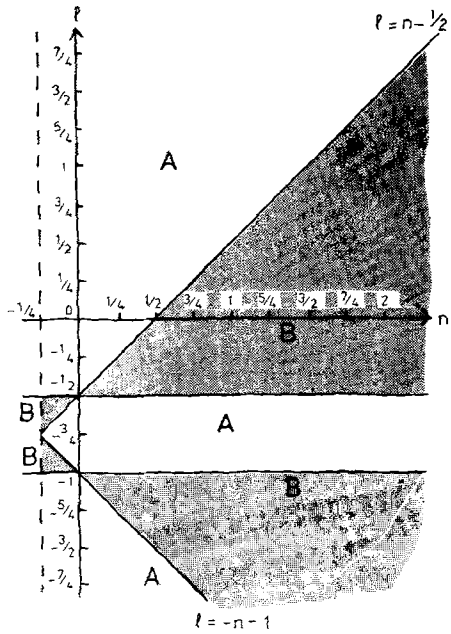

FIG. 1(a). The (l,n) plane for $n \geqslant -\frac{1}{4}$. The diagonal lines $l = n - \frac{1}{2}$ and $l = -n - 1$ represent possible maximum l-values within a star I.R. For the shaded regions labelled by A, $(l + m + 1) \geqslant 0$ and $(l - m) \leqslant 0$, whereas in the shaded regions labelled by B, $(l + m + 1) \leqslant 0$ and $(l - m) \geqslant 0$. On the boundary lines between the regions, the sign of $(l + m + 1)$ is arbitrary but opposite to the sign of $(l - m)$.

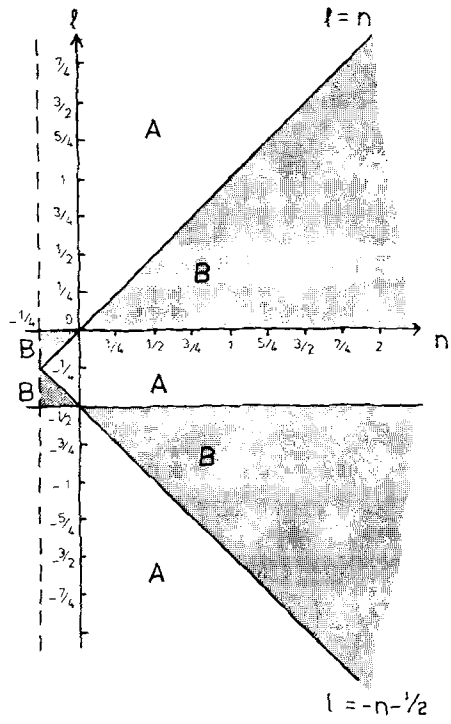

FIG. 1(b). Here the diagonal lines $l = n$ and $l = -n - \frac{1}{2}$ represent possible minimum l-values within a star I.R. For the shaded regions labelled by A, $(l + m) \geqslant 0$, and $(l - m + 1) \leqslant 0$, whereas in the shaded regions labelled by B, $(l + m) \leqslant 0$ and $(l - m + 1) \geqslant 0$. On the boundary lines between the regions, the sign of $(l + m)$ is arbitrary but opposite to the sign of $(l - m + 1)$.

and $l_- l_+$ have real nonpositive values, i.e. that $(l - m)(l + m + 1) \leqslant 0$ and $(l + m)(l - m + 1) \leqslant 0$. Also within an I.R. of Sl(2) the only possible minimum and maximum m values are $\underline{m} = -l$ or $(l + 1)$ and $\bar{m} = l$ or $-(l + 1)$. The classification of the star I.R.'s of $C(\mathrm{Sl}(2) \wedge T_2)$ therefore amounts to solving the (l,n) and (l,m) inequalities making use of the possible maximum and minimum values of l for fixed n and of m for fixed l.

This is achieved with the help of Figs. 1(a) and 1(b), in which the (l,n) plane is divided into regions A and B. In Fig. 1(a), $(l + n + 1)(2l - 2n + 1)(2l + 1)(l + 1)^{-1}$ is positive in region A, negative in region B, and vanishes on the lines $l = n - \frac{1}{2}$ and $l = -n - 1$, which are lines of maximum l. Hence in region A, $(l + m + 1) \geqslant 0$ and $(l - m) \leqslant 0$ and in region B, $(l + m + 1) \leqslant 0$ and $(l - m) \geqslant 0$, except on the dividing lines between the regions where the sign of $(l + m + 1)$ is arbitrary and opposite to that of $(l - m)$. In Fig. 1(b), $(l - n)(2l + 2n + 1)(2l + 1)l^{-1}$ is positive in region A, negative in region B, and vanishes on the lines $l = n$ and $l = -n - \frac{1}{2}$, which are lines of minimum l. Thus in region A, $(l + m) \geqslant 0$ and $(l - m + 1) \leqslant 0$ and in region B, $(l + m) \leqslant 0$ and $(l - m + 1) \geqslant 0$, except on the dividing lines between the regions where the sign of $(l + m)$ is arbitrary and opposite to that of $(l - m + 1)$.

Now in a BA region, [i.e., a region in the (l,n) plane of overlap between a B region of Fig. 1(a) and an A region of Fig. 1(b)] we must have both $(l + m + 1) \leqslant 0$ and $(l + m) \geqslant 0$, which is impossible; on the other hand, in an AB region we must have for all m values within an Sl(2)I.R., $(l + m + 1) \geqslant 0$ and $(l + m) \leqslant 0$, which is also impossible since the star I.R.'s of Sl(2) all have an infinite number of m-values differing by integral amounts. Hence AB and BA regions are forbidden territory for the l values within an I.R. of $C(\mathrm{Sl}(2) \wedge T_2)$ labelled by n.

The (l,m) inequalities show that, within an AA region, m must have a minimum value, so an I.R. of $C(\mathrm{Sl}(2) \wedge T_2)$ with l values in an AA region contains only the positive discrete type Sl(2) I.R.'s, i.e., D^+'s. On the other hand, for l values in a BB region, only the negative discrete D^- I.R.'s of Sl(2) are permitted. In fact, as we shall see, no I.R.'s containing D^-'s can occur. This, essentially, is due to the fact that, for fixed n, one cannot have l-values in a BB region without of necessity incurring l-values in an AB or BA region, where the star conditions are violated, but if l-values occur in an AA region, they can stop at the minimum $l = n$ line without entering the BA region, or they can stop at the maximum $l = -n - 1$ line without entering the AB region. If $n > \frac{1}{4}$, this is easy to see. First note that $\underline{l} = 0$ or $\bar{l} = -1$ are not possible since the matrix elements are singular at these points. An I.R. with $l = n, n + \frac{1}{2}, n + 1, \cdots$ is obviously possible, and this contains D^+'s with $\underline{m} = (l + 1)$; also an I.R. with $l = -(n + 1), -(n + \frac{1}{2}), -(n + 2), \cdots$ can occur, and this contains D^+'s with $\underline{m} = -l$. These I.R.'s are, however, equivalent due to the symmetry of $L^2 = l(l + 1)$ under $l \to -(l + 1)$, and since one conventionally chooses $l \geqslant 0$ for the I.R.'s of the compact SU(2) algebra and $l < 0$ for those of Sl(2), we shall choose $C(\mathrm{Sl}(2) \wedge T_2)$ I.R.'s, denoted Γ_1, to consist of $l = -(n + 1), -(n + \frac{1}{2}), -(n + 2), \cdots D^+$'s with $\underline{m} = -l$. These are the "mainstream" I.R.'s of $C(\mathrm{Sl}(2) \wedge T_2)$ and, as we shall see, occur for all values of n, even including $-\frac{1}{4} \leqslant n \leqslant \frac{1}{4}$. Clearly, for $n > \frac{1}{4}$, an I.R. with $\underline{l} = -n - \frac{1}{2}$ cannot occur since such an I.R. would contain $l = -n$, which is

in a BA region; for similar reasons we cannot have an I.R. with $\underline{l} = n - \frac{1}{2}$. Thus $\Gamma_{\rm I}$ are the only $C(\mathrm{Sl}(2) \wedge T_2)$ star I.R.'s which occur for $n > \frac{1}{4}$.

If $n < \frac{1}{4}$, the situation becomes more complicated. If $-\frac{1}{4} < n < 0$ or $0 < n < \frac{1}{4}$, in addition to the $\Gamma_{\rm I}$ I.R.'s, we also now have I.R.'s for which $l = -n - \frac{1}{2}, -n, -n + \frac{1}{2}, \cdots$ which contain D^+'s with $\underline{m} = (l + 1)$ and I.R.'s with $l = n - \frac{1}{2}, n - 1, n - \frac{3}{2}, \cdots$ which contain D^+'s with $\underline{m} = -l$. These are again equivalent so we get just a single extra class of I.R.'s, $\Gamma_{\rm II}$ with $l = n - \frac{1}{2}, n - 1, n - \frac{3}{2}, \cdots$ and $\underline{m} = -l$. For $n = -\frac{1}{4}$, $\Gamma_{\rm II}$ also exists but is identical to $\Gamma_{\rm I}$. It might appear for $-\frac{1}{4} \leqslant n < \frac{1}{4}$ that it is possible to get I.R.'s with no maximum or minimum l-values, but they are not in fact star I.R.'s since the m values for $l < -\frac{1}{2}$ states cannot be connected via the $p_{\pm\frac{1}{2}}$ to the m values for $l > -\frac{1}{2}$ states since they do not differ by multiples of $\frac{1}{2}$. If $n = 0$, $\Gamma_{\rm I}$ has $\underline{l} = -1$, but in this case the matrix elements are not singular due to a cancellation of the l^{-1} term with the $(l - n)$ term, so $\Gamma_{\rm I}$ is permissible. This is the only star I.R. of $C(\mathrm{Sl}(2) \wedge T_2)$ which contains an $l = -1$ I.R. of Sl(2). However, for $n = 0$, $\Gamma_{\rm II}$ does not occur since the value $l = -\frac{1}{2}$ cannot occur together with $l = -1$ due to $l = -1$ being itself a maximum l-value.

If $n = \frac{1}{4}$, $\Gamma_{\rm I}$ again clearly exists. However $\Gamma_{\rm II}$ does not occur since $\underline{l} = -n - \frac{1}{2} = -\frac{3}{4}$ and $\underline{l} = n - \frac{1}{2} = -\frac{1}{4}$ now differ by $\frac{1}{2}$; instead we get the pathological metaplectic representation Γ_M which is "dispin", containing an $l = -\frac{3}{4}$, $\underline{m} = \frac{3}{4}$ D^+ and an $l = -\frac{1}{4}$, $\underline{m} = \frac{1}{4}$ D^+. The I.R. with $\underline{l} = -\frac{3}{4}$, $\underline{m} = \frac{1}{4}$ and $l = -\frac{1}{4}$, $\underline{m} = \frac{3}{4}$ also exists but, since $l(l + 1)$ is the same for $l = -\frac{3}{4}$ and $l = -\frac{1}{4}$, this I.R. is entirely equivalent to Γ_M.

To summarize, the full set of inequivalent I.R.'s of $C(\mathrm{Sl}(2) \wedge T_2)$ consists of the following:

$\Gamma_{\rm I}$: $n \geqslant -\frac{1}{4}$; $l = -n - 1, -n - \frac{3}{2}, -n - 2, \ldots$ D^+'s with $\underline{m} = -l$.

$\Gamma_{\rm II}$: $-\frac{1}{4} < n < 0, 0 < n < \frac{1}{4}$; $l = n - \frac{1}{2}, n - 1, n - \frac{3}{2}, \ldots D^+$'s with $\underline{m} = -l$.

Γ_M: $n = \frac{1}{4}$; $l = -\frac{3}{4}$ D^+ with $\underline{m} = -\frac{3}{4}$ and $l = -\frac{1}{4} D^+$ with $\underline{m} = \frac{1}{4}$.

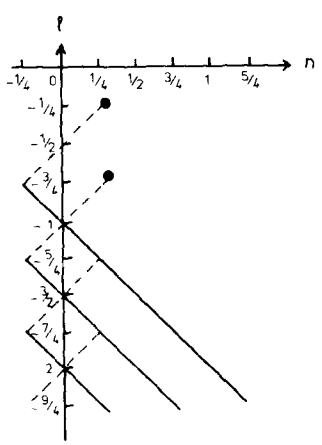

FIG. 2. The star I.R.'s of $C(\mathrm{Sl}(2) \wedge T_2)$ together with their Sl(2) content are depicted in the (l,n) plane. Points on unbroken lines are (l,n) values for $\Gamma_{\rm I}$, those on the broken lines are (l,n) values for $\Gamma_{\rm II}$; the circles correspond to Γ_M. The l-values contained in an I.R. labelled by n are connected vertically.

These I.R.'s are depicted in Fig. 2.

Note that, unlike the case of $\mathrm{Sl}(2) \wedge T_2$ itself, $C(\mathrm{Sl}(2) \wedge T_2)$ does not permit any I.R.'s which reduce to a single I.R. of Sl(2) with $p_{\pm\frac{1}{2}} = 0$ since such I.R.'s could not satisfy $[p_{\frac{1}{2}}, p_{-\frac{1}{2}}] = iI$. In particular, $C(\mathrm{Sl}(2) \wedge T_2)$ does not possess a trivial representation.

Using Eqs. (3.6) and (3.7) we may now calculate the actions of $O^{\pm\frac{1}{2},\pm\frac{1}{2}}$ on states $|n; l,m\rangle$ of an I.R.; with a suitable choice of relative phases of the states, we obtain

$$O^{\frac{1}{2},\frac{1}{2}}|n;l,m\rangle = \left[\frac{(l+m+1)(l+n+1)(2l-2n+1)(2l+1)}{2(l+1)}\right]^{1/2} \times |n;\, l+\tfrac{1}{2},\, m+\tfrac{1}{2}\rangle,$$

$$O^{-\frac{1}{2},-\frac{1}{2}}|n;l,m\rangle = i\left[\frac{(l+m)(l-n)(2l+2n+1)(2l+1)}{2l}\right]^{1/2} \times |n;\, l-\tfrac{1}{2},\, m-\tfrac{1}{2}\rangle.$$

From these one obtains

$$p_{\frac{1}{2}}|n;l,m\rangle = \left[\frac{(l+m+1)(l+n+1)(2l-2n+1)}{2(l+1)(2l+1)}\right]^{1/2} \times |n;\, l+\tfrac{1}{2},\, m+\tfrac{1}{2}\rangle - i\left[\frac{(m-l)(l-n)(2l+2n+1)}{2l(2l+1)}\right]^{1/2} \times |n;\, l-\tfrac{1}{2},\, m+\tfrac{1}{2}\rangle, \tag{3.8}$$

$$p_{-\frac{1}{2}}|n;\, l,m\rangle = \left[\frac{(m-l-1)(l+n+1)(2l-2n+1)}{2(l+1)(2l+1)}\right]^{1/2} \times |n;\, l+\tfrac{1}{2}, m-\tfrac{1}{2}\rangle - i\left[\frac{(l+m)(l-n)(2l+2n+1)}{2l(2l+1)}\right]^{1/2} \times |n;\, l-\tfrac{1}{2},\, m-\tfrac{1}{2}\rangle, \tag{3.9}$$

together with the Sl(2) actions

$$l_+|n;\, l,m\rangle = [(m-l)(l+m+1)]^{1/2}|n;\, l,m+1\rangle, \tag{3.10}$$

$$l_-|n;\, l,m\rangle = -[(l+m)(m-l-1)]^{1/2}|n;\, l,m-1\rangle. \tag{3.11}$$

Equations (3.8)–(3.11) are valid for all the I.R.'s, except for the $n = 0$ $\Gamma_{\rm I}$, where the actions of $p_{\pm\frac{1}{2}}$ on the $l = -1$ state become, instead of Eqs. (3.8) and (3.9),

$$p_{\frac{1}{2}}|0;-1,m\rangle = -i\,[(m+1)/2]^{1/2}|0;\, -\tfrac{1}{2}, m+\tfrac{1}{2}\rangle, \tag{3.12}$$

$$p_{-\frac{1}{2}}|0;-1,m\rangle = -i[(m-1)/2]^{1/2}|0;\, -\tfrac{1}{2}, m-\tfrac{1}{2}\rangle. \tag{3.13}$$

4. THE METAPLECTIC REPRESENTATION

Γ_M is the only "dispin" I.R. that $C(\mathrm{Sl}(2) \wedge T_2)$ possesses, and the only one it therefore possesses in common with the superalgebra Osp(2,1).[1] In order to compare Γ_M for the two algebras, we give the actions of $p_{\pm\frac{1}{2}}$ and $l_\pm$ explicitly. We represent the states by $|\frac{1}{4}; -\frac{3}{4}, \frac{3}{4} + S\rangle$ and $|\frac{1}{4}; -\frac{1}{4}, \frac{1}{4} + S\rangle$, where $S = 0,1,2,\ldots$. Eqs. (3.8)–(3.11) now become

$$p_{\frac{1}{2}}|\tfrac{1}{4};-\tfrac{3}{4},\tfrac{3}{4}+S\rangle=[2(S+1)]^{1/2}|\tfrac{1}{4};-\tfrac{1}{4},\tfrac{1}{4}+(S+1)\rangle, \tag{4.1}$$

$$p_{-\frac{1}{2}}|\tfrac{1}{4};-\tfrac{3}{4},\tfrac{3}{4}+S\rangle=[2S+1]^{1/2}|\tfrac{1}{4};-\tfrac{1}{4},\tfrac{1}{4}+S\rangle, \tag{4.2}$$

$$p_{1/2}|\tfrac{1}{4};-\tfrac{1}{4},\tfrac{1}{4}+S\rangle=-i[2S+1]^{1/2}|\tfrac{1}{4};-\tfrac{3}{4},\tfrac{3}{4}+S\rangle, \tag{4.3}$$

$$p_{-\frac{1}{2}}|\tfrac{1}{4};-\tfrac{1}{4},\tfrac{1}{4}+S\rangle=-i[2S]^{1/2}|\tfrac{1}{4};-\tfrac{3}{4},\tfrac{3}{4}+(S-1)\rangle, \tag{4.4}$$

$$l_+|\tfrac{1}{4};-\tfrac{3}{4},\tfrac{3}{4}+S\rangle=[(S+1)(2S+3)/2]^{1/2}\times|\tfrac{1}{4},-\tfrac{3}{4},\tfrac{3}{4}+(S+1)\rangle, \tag{4.5}$$

$$l_-|\tfrac{1}{4};-\tfrac{3}{4},\tfrac{3}{4}+S\rangle=-[S(2S+1)/2]^{1/2}\times|\tfrac{1}{4};-\tfrac{3}{4},\tfrac{3}{4}+(S-1)\rangle, \tag{4.6}$$

$$l_+|\tfrac{1}{4};-\tfrac{1}{4},\tfrac{1}{4}+S\rangle=[(S+1)(2S+1)/2]^{1/2}\times|\tfrac{1}{4};-\tfrac{1}{4},\tfrac{1}{4}+(S+1)\rangle, \tag{4.7}$$

$$l_-|\tfrac{1}{4};-\tfrac{1}{4},\tfrac{1}{4}+S\rangle=-[S(2S-1)/2]^{1/2}\times|\tfrac{1}{4};-\tfrac{1}{4},\tfrac{1}{4}+(S-1)\rangle. \tag{4.8}$$

Now for the metaplectic representation, $L^2=-\frac{3}{16}$, $I_3=\frac{3}{8}i$, so using Eq. (1.3), we see that $Y_+=-\frac{3}{4}i$. These are precisely the values obtained if $C(\mathrm{Sl}(2)\wedge T_2)$ is realized by

$$l_0=\tfrac{1}{2}zd/dz+\tfrac{1}{4}I,\quad l_+=\tfrac{1}{2}iz^2,\quad l_-=\tfrac{1}{2}id^2/dz^2, \tag{4.9}$$

$$p_{\frac{1}{2}}=-iz,\quad p_{-\frac{1}{2}}=d/dz, \tag{4.10}$$

[it is easy to check that these satisfy the commutation relations (1.1)]. Comparing these expressions with those obtained for the basis elements in the metaplectic representation of Osp(2,1) [Eqs. (5.9) and (5.10) of Hughes[1]], we see that the realizations of the metaplectic representations of $C(\mathrm{Sl}(2)\wedge T_2)$ and Osp(2,1) are connected by $q_{\pm\frac{1}{2}}=\frac{1}{2}e^{-i\pi/4}p_{\pm\frac{1}{2}}$; l_0 and l_+ have identical realizations for both algebras. The star conditions $p^\dagger_{\pm\frac{1}{2}}=ip_{\mp\frac{1}{2}}$ then correspond to $q^\dagger_{\pm\frac{1}{2}}=-q_{\mp\frac{1}{2}}$, the star conditions used for Osp(2,1). Finally, substituting for the $p_{\pm\frac{1}{2}}$ in terms of $q_{\pm\frac{1}{2}}$ in Eqs. (4.1)–(4.4) yields the actions of $q_{\pm\frac{1}{2}}$ on states of the metaplectic representation of Osp(2,1) as given in Eqs. (5.1)–(5.4) of Hughes,[1] except for phase factors. The difference in phase factors arises because of different conventions used for the relative phases of states within I.R.'s of $C(\mathrm{Sl}(2)\wedge T_2)$ and those of Osp(2,1).

In conclusion, we note that had we chosen for the I.R.'s of $C(\mathrm{Sl}(2)\wedge T_2)$ the star conditions $p^\dagger_{\pm\frac{1}{2}}=-ip_{\mp\frac{1}{2}}$, we should have obtained a similar classification of I.R.'s, except that instead of D^+'s only D^-'s would occur.

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Non-self-adjoint Zakharov–Shabat operator with a potential of the finite asymptotic values. I. Direct spectral and scattering problems

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(Received 2 December 1980; accepted for publication 12 June 1981)

The Zakharov and Shabat equation for the scattering problem is studied. The estimates, analytical properties, and asymptotic expansions of the Jost solution are presented for a general class of the potentials $Q(x)$ not vanishing at infinity. The existence of the similarity transformation is also shown. For $Q(x)$ vanishing at infinity, the continuous part of the spectrum doubly degenerates. However, nonvanishing (finite) asymptotic values of $Q(x)$ dissolve the degeneracy completely. The expansion theorem is given in $C_0^2(\mathbb{R})$ and for a class of $Q(x)$ we prove that the Zakharov and Shabat equation yields a non-self-adjoint spectral operator in the Hilbert space in the sense of Dunford and Schwartz.

PACS numbers: 02.30.Hq, 03.65.Nk, 03.65.Db

I. INTRODUCTION

Following the successful application to the Korteweg–de Vries equation,[1] the inverse scattering method[2,3] was employed to study classes of nonlinear evolution equations. Especially, Zakharov and Shabat[4] introduced a system of the differential equation

$$v_x = -i\lambda\sigma_3 v + Q(x)v, \tag{1.1}$$

$$v = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad Q(x) = \begin{pmatrix} 0 & q(x) \\ r(x) & 0 \end{pmatrix},$$

where λ, $Q(x) \in \mathbb{C}$ and $x \in \mathbb{R}$ and solved the nonlinear Schrödinger equation. Equation (1.1) was extensively studied by Ablowitz, Kaup, Newell, and Segur[5] and shown to yield the spectral problem relevant to the wide classes of evolution equations. We may regard it as an extended form of a one dimensional Dirac equation and, in fact, the direct and the inverse spectral problems of (1.1) under various conditions have been investigated historically as those in quantum mechanics. Gasymov and Levitan,[6] for example, discussed the inverse spectral problem of (1.1) on the half-axis $0 \leqslant x < \infty$ for the potentials satisfying the conditions

$$r = \bar{q}, \quad |\mathrm{Re}q| \leqslant \frac{c}{(1+x)^{1+\epsilon}}, \quad |\mathrm{Im}q| \leqslant \frac{c}{(1+x)^{2+\epsilon}},$$

where $\bar{q}$ is the complex conjugate of q and c and ϵ are positive constants. Ablowitz *et al.* studied (1.1) for the nonsymmetric potentials rapidly decreasing at infinity $x \to \pm\infty$. In order to obtain the solution of the nonlinear Schrödinger equation with the nonvanishing boundary values at infinity, Kawata and Inoue[7] considered (1.1) with the potentials not vanishing at infinity; $q \to q_\pm, r \to r_\pm$ as $x \to \pm\infty$ under the restriction $q_+ r_+ = q_- r_-$; here and henceforth $\pm$ signs are ordered.

We examine the direct and inverse spectral problem of (1.1) and the present paper deals with the direct spectral and scattering problems. It is worthwhile to note that the equation

$$v_x = -i\lambda\sigma_3 v + Q(x)v, \tag{1.2}$$

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad Q(x) = \begin{pmatrix} p(x) & q(x) \\ r(x) & s(x) \end{pmatrix}$$

can be reduced to (1.1) by the transformation

$$v \to \begin{pmatrix} e^{\int p dx} & 0 \\ 0 & e^{\int s dx} \end{pmatrix} v, \quad \begin{pmatrix} q \\ r \end{pmatrix} \to \begin{pmatrix} e^{\int (p-s)dx} & 0 \\ 0 & e^{\int (s-p)dx} \end{pmatrix} \begin{pmatrix} q \\ r \end{pmatrix}. \tag{1.3}$$

Throughout the paper, the asymptotic values of Q for $x \to \pm\infty$ are assumed to be constants $Q_\pm (\neq 0) \in \mathbb{C}$. In Sec. 2, the properties of the Jost solutions of (1.1) are studied and the correspondence of the functional spaces of the potentials and the Jost solutions are presented. The existence of the similarity transformation is also proved. In Sec. 3, the results of Sec. 2 are used to introduce the Green function and we obtain the expansion theorems for (1.1) together with the stability of the continuous spectrum under the perturbation of the potential. For $Q_\pm = 0$ the continuous spectrum degenerates. However, it is shown that the asymptotic condition $q_+ r_+ - q_- r_- \in \mathbb{C}(\notin \mathbb{R})$ dissolves the degeneracy completely. It is shown that the convergence of the expansion for the test function in $C_0^2(\mathbb{R})$ is uniform in each finite interval of $x \in \mathbb{R}$. In Sec. 4 we study the scattering matrix for the class of the asymptotic values of $Q_\pm, q_+ r_+ - q_- r_- \in \mathbb{R}$, and, in this case, investigate the spectral resolution of the operator L in the Hilbert space $H = \otimes (L^2(\mathbb{R}))^2$. Thus, the Zakharov–Shabat system (1.1) yields a non-self-adjoint spectral operator[8] solvable by means of the Jost solution method. For later use, we introduce some notations:

$$CF_\pm(n) \equiv \left\{ f(x) \,|\, f \in \mathbb{C}, \mp \int_{\pm\infty}^{x} dy (1 + |y|^n) |f(y)| < \infty, x \in \mathbb{R} \right\}, \quad n = 0, 1, \cdots,$$

$$CF'_\pm(n) \equiv \left\{ f(x) \,|\, f \in \mathbb{C}, \mp \int_{\pm\infty}^{x} (1 + |y|^n) |df(y)| < \infty, x \in \mathbb{R} \right\}, \quad n = 0, 1, \cdots.$$

The asymptotic values $f_\pm$ of $f(x)$ for $x \to \pm\infty$ are defined, if and only if $f_\pm(x) = f(x) - f_\pm \in CF_\pm(0)$ in the sense of the first definition. The second definition is given for f of bounded variation on the entire axis, $y \in \mathbb{R}$, and f is piecewise differentiable, $f'(y)$ existing except on a denumerable set of $y \in \mathbb{R}$, where $|df(y)| = |f(y+0) - f(y-0)|$. We note that if $f \in CF'_\pm(n+1)$ and $f_\pm = 0$, then $f \in CF'_\pm(n)$, and if $f \in CF'_\pm(0)$, then $|f(x) - f_\pm| < \mp \int_{\pm\infty}^{x \mp 0} |df(y)|$, and that $\int_x^{\pm\infty} dy (1 + |y|^n) |f(y)| \in CF_\pm(0)$

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and $\int_{\pm\infty}^{x}(1+|y|^n)|df(y)| \in CF_{\pm}(0)$ are equivalent to $f \in CF_{\pm}(n+1)$ and $f \in CF_{\pm}'(n+1)$, respectively. When each component of a matrix $F(x)$ belongs to the class $CF_{\pm}(n)$ or $CF_{\pm}'(n)$, we write it as $F(x) \in CF_{\pm}(n)$ or $F(x) \in CF_{\pm}'(n)$, respectively. Let $v=\{v_i\}$ and $M=\{M_{ij}\}$ be a vector and matrix, respectively, then we define a new vector and matrix with positive components;

$$|v| = \{|v|_i\}(|v|_i = |v_i|), \quad |M| = \{|M|_{ij}\}(|M|_{ij} = |M_{ij}|).$$

It is easy to see that

$$|Mv| \leqslant |M|\,|v|, \quad |MN| \leqslant |M|\,|N|, \text{ etc.},$$

where inequalities $|v| < |w|$ and $|M| < |N|$ mean $|v_i| \leqslant |w_i|(|v| \neq |w|)$ and $|M_{ij}| \leqslant |N_{ij}|(|M| \neq |N|)$, respectively.

2. PROPERTIES OF THE JOST SOLUTION

In the standard form of the spectral problem, (1.1) is written in the form

$$Lv = \lambda v, \tag{2.1}$$

$$L = i\sigma_3 \frac{\partial}{\partial x} - i\sigma_3 Q. \tag{2.2}$$

The Jost solutions $\phi_{\pm 1}(x,\lambda,\lambda_{\pm})$ and $\phi_{\pm 2}(x,\lambda,\lambda_{\pm})$ of (2.1) are the linearly independent solutions specified by the boundary conditions

$$\phi_{\pm 1} \sim \begin{pmatrix} e^{-i\lambda_{\pm} x} \\ 0 \end{pmatrix}, \quad \phi_{\pm 2} \sim \begin{pmatrix} 0 \\ e^{i\lambda_{\pm} x} \end{pmatrix}, \quad x \to \pm\infty,$$

where $\lambda_{\pm} = (\lambda^2 - u^2_{\pm})^{1/2} \in \mathbb{R}, u^2_{\pm} = q_{\pm} r_{\pm} \in \mathbb{C}$. The matrix Jost solution $\Phi_{\pm}(x,\lambda,\lambda_{\pm})$ for $\lambda_{\pm} \in \mathbb{R}$ is defined by the solution of (2.1) satisfying the condition

$$\begin{aligned} &\Phi_{\pm}(x,\lambda,\lambda_{\pm}) \to \Phi_{\pm}^{(0)}(x,\lambda,\lambda_{\pm}), \quad x \to \pm\infty, \\ &\Phi_{\pm}^{(0)}(x,\lambda,\lambda_{\pm}) = T_{\pm}(\lambda,\lambda_{\pm}) J(x,\lambda_{\pm}), \end{aligned} \tag{2.3}$$

where

$$T_{\pm}(\lambda,\lambda_{\pm}) = \begin{pmatrix} 1 & -iq_{\pm}/(\lambda+\lambda_{\pm}) \\ ir_{\pm}/(\lambda+\lambda_{\pm}) & 1 \end{pmatrix},$$

$$J(x,\lambda_{\pm}) = \begin{pmatrix} e^{-i\lambda_{\pm} x} & 0 \\ 0 & e^{i\lambda_{\pm} x} \end{pmatrix}.$$

The vector solutions $\phi_{\pm 1}$ and $\phi_{\pm 2}$ are chosen so as to constitute $\Phi_{\pm}$ in the form $\Phi_{\pm} = (\phi_{\pm 1}, \phi_{\pm 2})$. Our analysis of the Jost solution is based on the integral equation equivalent to (2.1) and (2.3),

$$\Phi_{\pm}(x,\lambda,\lambda_{\pm}) = \Phi_{\pm}^{(0)}(x,\lambda,\lambda_{\pm}) + \int_{\pm\infty}^{x} dy\, V_{\pm}(x,y,\lambda,\lambda_{\pm}) \times \Phi_{\pm}(y,\lambda,\lambda_{\pm}), \tag{2.4}$$

where the kernel is given by

$$V_{\pm}(x,y,\lambda,\lambda_{\pm}) = \Phi_{\pm}^{(0)}(x,\lambda,\lambda_{\pm}) \Phi_{\pm}^{(0)}(y,\lambda,\lambda_{\pm})^{-1} \times \tilde{Q}_{\pm}(y), \tag{2.5}$$

$$\Phi_{\pm}^{(0)}(x,\lambda,\lambda_{\pm}) \Phi_{\pm}^{(0)}(y,\lambda,\lambda_{\pm})^{-1} = \frac{1}{\lambda_{\pm}} \times \begin{pmatrix} \lambda_{\pm}\cos Z_{\pm} - i\lambda \sin Z_{\pm} & q_{\pm}\sin Z_{\pm} \\ r_{\pm}\sin Z_{\pm} & \lambda_{\pm}\cos Z_{\pm} + i\lambda \sin Z_{\pm} \end{pmatrix},$$

$$\tilde{Q}_{\pm}(y) = Q(y) - Q_{\pm}, \quad Z_{\pm} = \lambda_{\pm}(x-y).$$

Later we must examine the analytical properties of the functions of λ, λ_+, and λ_-. The Riemann surface for the pair λ_+ and λ_- generally consists from four sheets R_J (J = I–IV) according to the signs of $(\lambda^2 - u^2_+)^{1/2}$ and $(\lambda^2 - u^2_-)^{1/2}$. We define the first sheet of R, R_I, such that $\lambda_{\pm} \sim \lambda$ as $|\lambda| \to \infty$ on it. An example of R_I is shown in Fig. 1 for the special case where both of $u_{\pm}$ ($|u_+| > |u_-| > 0, \arg u_+ < \arg u_-$) are on the first quadrant. R_I has two branch cuts between $u_{\pm}$ and $-u_{\pm}$ and it is convenient for later discussions to define one of them so as to include the other as a part and to be symmetric with respect to the origin $\lambda = 0$, as shown in Fig. 1 by the dotted curves Γ, Γ' ($\Gamma = \Gamma' + \Lambda_+ + \Lambda_-$). The curves C_1, C_4 and C_2, C_3 are the loci corresponding to $\nu_{\pm} = \mathrm{Im}\lambda_{\pm} = 0$, respectively, and are the parts of the rectangular hyperbolas $\xi\eta = \mathrm{Re}u_{\pm}\,\mathrm{I}m u_{\pm}$ ($\lambda = \xi + i\eta$). Thus, R_I is divided into four regions by these curves and branch cuts; $R_1(\nu_{\pm} > 0)$, $R_2(\nu_+ < 0, \nu_- > 0)$, $R_3(\nu_+ > 0, \nu_- < 0)$, and $R_4(\nu_{\pm} < 0)$. Similar curves may be drawn for other conditions on $u_{\pm}$. It is clear that, without loss of generality, we may assume $\mathrm{Re}u_{\pm} > 0$. In Sec. 3 it will be shown that the totality of the curves C_i constitutes the continuous part of the spectrum of (2.1). Each of the remaining sheets R_{II}, R_{III}, R_{IV} has the same branch cuts Γ, Γ' and curves C_1–C_4 and, hence, the same regions R_1–R_4 as R_I. In this paper we study various functions of $\{\lambda, \lambda_+, \lambda_-\}$ exclusively on R_I and identify the complex λ plane to R_I. First of all, we analyticaly continue the Jost solution $\Phi_{\pm}(x,\lambda,\lambda_{\pm})$ of (2.1) with its boundary condition (2.3) defined only for $\lambda_{\pm} \in \mathbb{R}$. Let D be the region in R_I where the Jost solution, as well as the boundary condition, can be continued. Employing the same notations as before, we have the boundary condition for $\lambda \in D$,

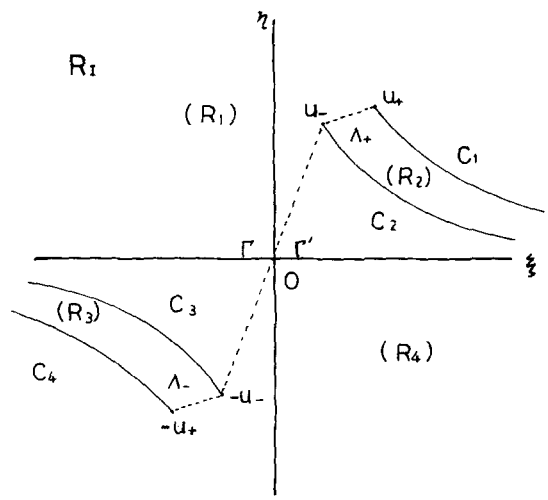

FIG. 1. The first Riemann sheet and branch cuts.

$$\phi_{\pm 1}(x,\lambda,\lambda_{\pm}) \to \phi_{\pm 1}{}^{(0)}(x,\lambda,\lambda_{\pm}) = T_{\pm}(\lambda,\lambda_{\pm}) \begin{pmatrix} e^{-i\lambda_{\pm} x} \\ 0 \end{pmatrix},$$
$$x \to \pm\infty \quad \text{for } \nu_{\pm} \lesseqgtr 0, \tag{2.6}$$
$$\phi_{\pm 2}(x,\lambda,\lambda_{\pm}) \to \phi_{\pm 2}{}^{(0)}(x,\lambda,\lambda_{\pm}) = T_{\pm}(\lambda,\lambda_{\pm}) \begin{pmatrix} 0 \\ e^{i\lambda_{\pm} x} \end{pmatrix},$$
$$x \to \pm\infty \quad \text{for } \nu_{\pm} \gtreqless 0.$$

They are, if they exist, the single valued functions of λ and might better be written as $\phi_{\pm j}(x,\lambda,\lambda_{\pm}(\lambda))$ as well as the single valued functions $\phi_{\pm j}{}^{(0)}(x,\lambda,\lambda_{\pm}(\lambda))(\lambda \in R_{\mathrm{I}})$. We, however, omit variables $\lambda, \lambda_{\pm}$ frequently for brevity. Instead of (2.4), we examine the integral equation

$$\phi_{\pm j}(x) = \phi_{\pm j}{}^{(0)}(x) + \int_{\pm\infty}^{x} dy\, V_{\pm}(x,y)\phi_{\pm j} \quad (j = 1,2), \tag{2.7}$$

where

$$\nu_{\pm} \lesseqgtr 0 \quad \text{for } j = 1, \quad \nu_{\pm} \gtreqless 0 \quad \text{for } j = 2$$

and $V_{\pm}(x,y)$ is given by (2.5) for $\lambda \in R_{\mathrm{I}}$. Each of (2.7) is equivalent to (2.1) with the condition (2.6).

Lemma 1: Let $\tilde{Q}_{\pm} \in CF_{\pm}(0)$, then $\phi_{\pm 1}$ and $\phi_{\pm 2}$ are analytic in the half-plane $\nu_{\pm} \lesseqgtr 0$ and $\nu_{\pm} \gtreqless 0$ of R_{I}, respectively, and $\Phi_{\pm} = (\phi_{\pm 1}, \phi_{\pm 2})$ is continuous in λ on the curve corresponding to $\nu_{\pm} = 0$ except at $\lambda = \pm u_{\pm}, \mp u_{\pm}$, which corresponds to $\lambda_{\pm} = 0$. We have the estimates for $\lambda_{\pm} \neq 0$,

$$\begin{Bmatrix} |\phi_{\pm 1}(x)| \\ |\phi_{\pm 2}(x)| \end{Bmatrix} < (1+\alpha_{\pm}) \begin{pmatrix} 1 \\ 1 \end{pmatrix} e^{\beta_{\pm} I_{\pm}(x)} \begin{Bmatrix} e^{\nu_{\pm} x} \\ e^{-\nu_{\pm} x} \end{Bmatrix}, \begin{Bmatrix} \nu_{\pm} \lesseqgtr 0 \\ \nu_{\pm} \gtreqless 0 \end{Bmatrix}, \tag{2.8}$$

where $\alpha_{\pm}$ and $\beta_{\pm}$ are constants depending on λ, $\lambda_{\pm}$, and $Q_{\pm}$, and

$$I_{\pm}(x) = \mp \int_{\pm\infty}^{x} dy(|\tilde{q}_{\pm}(y)| + |\tilde{r}_{\pm}(y)|). \tag{2.9}$$

Further, let $\tilde{Q}_{\pm} \in CF_{\pm}(1)$, then $\Phi_{\pm}$ is continuous even at $\lambda = \pm u_{\pm}, \mp u_{\pm}$ and has the continuous first derivative in λ along the curve $\nu_{\pm}(\lambda) = 0 (\lambda_{\pm} \neq 0)$.

Proof: Let us introduce $\psi_{\pm j}(x)$ by

$$\phi_{\pm j} = \Phi_{\pm}{}^{(0)}(x) U_{\pm}(x) \psi_{\pm j}(x), \quad j = 1,2 \tag{2.10}$$

where

$$U_{\pm}(x) = \begin{pmatrix} e^{(i/2)i\theta_{\pm}} & 0 \\ 0 & e^{-(1/2)i\theta_{\pm}} \end{pmatrix},$$
$$\theta_{\pm}(x,\lambda_{\pm}) = \frac{1}{\lambda_{\pm}} \int_{\pm\infty}^{x} dy(q_{\pm}\tilde{r}_{\pm}(y) + r_{\pm}\tilde{q}_{\pm}(y)).$$

Then, (2.7) is transformed to the integral equation for $\psi_{\pm j}$;

$$\psi_{\pm j}(x) = \begin{pmatrix} \delta_{1j} \\ \delta_{2j} \end{pmatrix} + \int_{\pm\infty}^{x} dy\, W_{\pm}(y)\psi_{\pm j}(y), \quad j = 1,2 \tag{2.11}$$

with the kernel

$$W_{\pm}(x,\lambda,\lambda_{\pm}) = \frac{\lambda+\lambda_{\pm}}{2\lambda_{\pm}} \begin{pmatrix} 0 & \hat{q}_{\pm}(x) e^{i(2\lambda_{\pm} x - \theta_{\pm})} \\ \hat{r}_{\pm}(x) e^{-i(2\lambda_{\pm} x - \theta_{\pm})} & 0 \end{pmatrix}, \tag{2.12}$$

where δ_{ij} is Kronecker's delta and

$$\hat{q}_{\pm}(x,\lambda,\lambda_{\pm}) = \tilde{q}_{\pm}(x) + \left(\frac{q_{\pm}}{\lambda+\lambda_{\pm}}\right)^2 \tilde{r}_{\pm}(x), \qquad \hat{r}_{\pm}(x,\lambda,\lambda_{\pm}) = \tilde{r}_{\pm}(x) + \left(\frac{r_{\pm}}{\lambda+\lambda_{\pm}}\right)^2 \tilde{q}_{\pm}(x).$$

The integral equation (2.11) is of the Volterra type and the Neumann series for $\psi_{\pm j}$ is given formally as

$$\psi_{\pm j}(x) = \sum_{n=0}^{\infty} \psi_{\pm j}{}^{(n)}, \tag{2.13}$$
$$\psi_{\pm j}{}^{(0)} = \begin{pmatrix} \delta_{1j} \\ \delta_{2j} \end{pmatrix},$$
$$\psi_{\pm j}{}^{(n)}(x) = \int_{\pm\infty}^{x} dx_1\, W_{\pm}(x_1)\psi_{\pm j}{}^{(n-1)}(x_1) = \int_{\pm\infty}^{x} dx_1 \int_{\pm\infty}^{x_1} dx_2 \cdots \int_{\pm\infty}^{x_{n-1}} dx_n\, W_{\pm}(x_1)W_{\pm}(x_2)\cdots W_{\pm}(x_n)\psi_{\pm j}(0),$$

$n \geqslant 1$.

We show the details of the calculation only for $\psi_{\pm 1}$;

$$\psi_{\pm 1}{}^{(2m)}(x) = \left(\frac{\lambda+\lambda_{\pm}}{2\lambda_{\pm}}\right)^{2m} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \int_{\pm\infty}^{x} dx_1 \int_{\pm\infty}^{x_1} dx_2 \cdots \int_{\pm\infty}^{x_{2m-1}} dx_{2m}\, \hat{q}_{\pm}(x_1)\hat{r}_{\pm}(x_2)\cdots\hat{q}_{\pm}(x_{2m-1})\hat{r}_{\pm}(x_{2m})$$
$$\times e^{2i\lambda_{\pm}(x_1 - x_2 + \cdots - x_{2m}) - i(\theta_{\pm}(x_1) - \theta_{\pm}(x_2) + \cdots - \theta_{\pm}(x_{2m}))}, \tag{2.14a}$$

$$\psi_{\pm 1}{}^{(2m-1)}(x) = \left(\frac{\lambda+\lambda_{\pm}}{2\lambda_{\pm}}\right)^{2m-1} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \int_{\pm\infty}^{x} dx_1 \int_{\pm\infty}^{x_1} dx_2 \cdots \int_{\pm\infty}^{x_{2m-2}} dx_{2m-1}\, \hat{r}_{+}(x_1)\hat{q}_{+}(x_2)\cdots\hat{q}_{\pm}(x_{2m-2})\hat{r}_{\pm}(x_{2m-1})$$
$$\times e^{2i\lambda_{\pm}(-x_1 + x_2 \cdots - x_{2m-1}) - i(-\theta_{\pm}(x_1) + \theta_{\pm}(x_2) - \cdots - \theta_{\pm}(x_{2m-1}))}, \quad (m \geqslant 1). \tag{2.14b}$$

Then $\psi_{+1}{}^{(n)}$ exists and the estimates

$$|\psi_{\pm 1}{}^{(2m)}(x)| \leqslant \begin{pmatrix} 1 \\ 0 \end{pmatrix} \frac{1}{(2m)!} \{g_{\pm}(x)\}^{2m} e^{h_{+}(x)},$$

$$|\psi_{\pm 1}{}^{(2m-1)}(x)| \leqslant \binom{0}{1} \frac{1}{(2m-1)!}\{g_\pm(x)\}^{2m-1} e^{h_\pm(x)+2\nu_\pm x},$$

hold for $\nu_\pm \lesseqgtr 0$, where

$$g_\pm(x,\lambda,\lambda_\pm) = \mp \left|\frac{\lambda+\lambda_\pm}{2\lambda_\pm}\right| \int_{\pm\infty}^{x} dy\{|\hat{q}_\pm(y,\lambda,\lambda_\pm)| + |\hat{r}_\pm(y,\lambda,\lambda_\pm)|\},$$

$$h_\pm(x,\lambda,\lambda_\pm) = \mp \int_{\pm\infty}^{x} dy \frac{1}{|\lambda_\pm|}\{|q_\pm \tilde{r}_\pm(y)| + |r_\pm \tilde{q}_\pm(y)|\}. \tag{2.15}$$

For $\tilde{Q}_\pm \in CF_\pm(0)$, we have $I_\pm(x) < \infty$ for $x \in [x_0, \mp\infty)$, $(x_0 \in R)$,

$$g_\pm \leqslant \left|\frac{\lambda+\lambda_\pm}{2\lambda_\pm}\right| (1+\alpha_\pm^2) I_\pm(x), \quad \left(\alpha_\pm = \frac{|q_\pm| + |r_\pm|}{|\lambda+\lambda_\pm|}\right), \quad h_\pm \leqslant \left|\frac{\lambda+\lambda_\pm}{\lambda_\pm}\right| \alpha_\pm I_\pm(x), \tag{2.16}$$

and

$$|\psi_{\pm 1}(x)| < \begin{pmatrix} 1 \\ e^{2\nu_\pm x} \end{pmatrix} e^{g_\pm(x)+h_\pm(x)}. \tag{2.17}$$

From (2.16), (2.17), (2.10), (2.6), and (2.3) one has (2.8) with

$$\beta_\pm = \frac{|\lambda+\lambda_\pm|}{2|\lambda_\pm|}(1+5\alpha_\pm+\alpha_\pm{}^2).$$

Since the convergence of (2.14) is uniform in each bounded region of $x \in \mathbb{R}$ and $\nu_+(\lambda) \leqslant 0$ except in the vicinity of $\lambda_+ = 0$, ψ_{+1} and hence $\phi_{+1} = \Phi_+{}^{(0)} U_+ \psi_{+1}$ is analytic in λ for $\nu_+ < 0$ and continuous for $\nu_+ \leqslant 0$ $(\lambda_+ \neq 0)$. The continuous differentiability of $\phi_{\pm j}$ with respect to λ along the curve $\lambda_\pm(\lambda) \in \mathbb{R}$ is also obtained under the stronger assumption, $\tilde{Q}_\pm \in CF_\pm(1)$. Indeed, the differentiation of $\psi_{+1}{}^{(n)}(x)$ of (2.14) with respect to λ_+ (or λ) yields the factor x_j from $\exp[i\lambda_+ x_j]$ which is, however, integrated and estimated with slight modification of the case $\tilde{Q}_\pm \in CF_\pm(0)$. Further, one may construct the Neumann series representation of $\phi_{\pm j}$ from the original integral equation (2.7) instead of (2.11). Then, due to the inequality $|\cos Z|$, $|\sin Z/Z| \leqslant e^{|\mathrm{Im} Z|}$, one has $V_\pm \in CF_\pm(0)$ for each fixed $x, \lambda, \lambda_\pm(\lambda)$ and the absolute and uniform convergence of the series even in the vicinity of $\lambda_\pm = 0$. Hence $\phi_{\pm 1}$ is continuous at $\lambda = \pm u_\pm, \mp u_\pm$. The discussions go parallel with $\phi_{\pm 1}$ for $\phi_{\pm 2}$ and we omit them. Q.E.D.

Asymptotic behaviors of $\phi_{\pm j}(x)(j = 1,2)$ can be seen by Lemma 1. However, we can give the more efficient estimate and asymptotic forms for large $|\lambda|$ as well.

Lemma 2. Let $\tilde{Q}_+ \in CF_\pm(0) \cap CF'_\pm(0)$, then we have the estimate

$$\left\{\begin{array}{l} \left|\phi_{\pm 1} e^{i\lambda_\pm x} - \begin{pmatrix} 1 \\ \dfrac{ir_\pm}{\lambda+\lambda_\pm} \end{pmatrix}\right| \\ \left|\phi_{\pm 2} e^{-i\lambda_+ x} - \begin{pmatrix} \dfrac{-iq_\pm}{\lambda+\lambda_\pm} \\ 1 \end{pmatrix}\right| \end{array}\right\} < \frac{1}{|\lambda_\pm|}\gamma_\pm \begin{pmatrix} 1 \\ 1 \end{pmatrix} [J_\pm(x) + |\lambda_\pm|\alpha_\pm^2 I_\pm(x)] e^{\beta_\pm I_+(x)} \quad \text{for} \begin{Bmatrix} \nu_\pm \lesseqgtr 0 \\ \nu_\pm \gtreqless 0 \end{Bmatrix}, \tag{2.18}$$

where $\gamma_\pm$ is a constant such that $\gamma_\pm \to 1$ as $|\lambda| \to \infty$ and $J_\pm(x)$ is defined by

$$J_\pm(x) = \mp \int_{\pm\infty}^{x} (|dq(y)| + |dr(y)|). \tag{2.19}$$

The asymptotic form of the Jost solution is given as

$$\phi_{\pm 1} e^{i\lambda_\pm x} - \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{i}{2\lambda_\pm}\begin{pmatrix} \pi_\pm(x) \\ r(x) \pm \sum\limits_{x_j \gtreqless x}^{n} \delta r_j e^{2i\lambda_\pm(x-x_j)} \end{pmatrix} + o(|\lambda|^{-1}), \quad \nu_\pm \lesseqgtr 0,$$

$$\phi_{\pm 2} e^{-i\lambda_\pm x} - \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{-i}{2\lambda_\pm}\begin{pmatrix} q(x) \pm \sum\limits_{x_j \gtreqless x}^{n} \delta q_j e^{-2i\lambda_\pm(x-x_j)} \\ \pi_\pm(x) \end{pmatrix} + o(|\lambda|^{-1}), \quad \nu_\pm \gtreqless 0, \tag{2.20}$$

to the order $|\lambda|^{-1}$ uniformly for $x\in[x_0, \pm\infty)$,$(x_0\in\mathbb{R})$, where

$$\pi_{\pm}(x) = \int_{\pm\infty}^{x} dy\{q(y)r(y) - q_{\pm}r_{\pm}\}.$$

The summation $\Sigma^{n}_{x_j\gtrless x}$ should be taken under the restriction $x_j\gtrless x$ at $\{x_j|j=1,\cdots,n\leqslant\infty\}$, where $\tilde{Q}_{\pm}(x)\in CF'_{\pm}(0)$ makes leaps $\begin{pmatrix}0 & \delta q_j\\ \delta r_j & 0\end{pmatrix}$.

Proof: Let $\Sigma_{\pm j}(j=1,2)$ be the right hand side of (2.13) subtracted the first term, then we have, from (2.3) and (2.10),

$$\phi_{\pm 1}e^{i\lambda_{+}x} - \begin{pmatrix}1\\ \dfrac{ir_{\pm}}{\lambda+\lambda_{\pm}}\end{pmatrix} = \Phi_{\pm}{}^{(0)}U_{\pm}e^{i\lambda_{+}x}\left[\Sigma_{\pm 1} + \begin{pmatrix}1\\0\end{pmatrix}(1-e^{-(i/2)\theta_{+}})\right]. \tag{2.21}$$

In (2.14), the integrations by parts in x_{2m} or x_{2m-1} yield new series containing $\lambda_{\pm}^{-1}$ as a factor and we have the estimate

$$|\psi_{\pm 1}{}^{(2m)}(x)| \leqslant \frac{1}{|\lambda_{\pm}|}e^{h_{+}(x)}\begin{pmatrix}1\\0\end{pmatrix}\left[(1+\alpha_{\pm}{}^{2})\frac{1}{(2m-1)!}g_{\pm}(x)^{2m-1} + \alpha_{\pm}\frac{1}{(2m)!}g_{\pm}(x)^{2m}\right]\left|\frac{\lambda+\lambda_{\pm}}{2\lambda_{\pm}}\right|J_{\pm}(x) \quad (\nu_{\pm}\lesseqgtr 0),$$

$$|\psi_{\pm 1}{}^{(2m-1)}(x)| \leqslant \frac{1}{|\lambda_{\pm}|}e^{h_{+}(x)+2\nu_{\pm}x}\begin{pmatrix}0\\1\end{pmatrix}\left[(1+\alpha_{\pm}{}^{2})\frac{1}{(2m-2)!}g(x)^{2m-2} + \alpha_{\pm}\frac{1}{(2m-1)!}g_{\pm}(x)^{2m-1}\right]\left|\frac{\lambda+\lambda_{\pm}}{2\lambda_{\pm}}\right|J_{\pm}(x)$$

$$(\nu_{\pm}\lesseqgtr 0);$$

here $g_{\pm}(x)$ and $h_{\pm}(x)$ are given by (2.15), and

$$|\Sigma_{\pm 1}| \leqslant \frac{|\lambda+\lambda_{\pm}|}{2|\lambda_{\pm}|^{2}}(1+\alpha_{\pm}+\alpha_{\pm}{}^{2})e^{g_{\pm}(x)+h_{\pm}(x)}\begin{pmatrix}1\\e^{2\nu_{\pm}x}\end{pmatrix}J_{\pm}(x).$$

Substituting the last inequality and $|1-e^{z}|\leqslant|z|e^{|z|}$ into (2.21) and estimating $g_{\pm}(x)$, $h_{\pm}(x)$, and so on, we have the first inequality of (2.18) with $\gamma_{\pm}$ given by

$$\gamma_{\pm} = \tfrac{1}{2}(1+|\lambda/\lambda_{\pm}|)(1+\alpha_{\pm})(1+\alpha_{\pm}+\alpha_{\pm}{}^{2}).$$

The second inequality of (2.18) is obtained likewise and hence the first half of the lemma is proved. The asymptotic expansion (2.20) for $\phi_{\pm 1}$ is obtained from that of the right hand side of (2.21). Integrating by parts once in (2.14) and using the Riemann–Lebesgue theorem to evaluate each order of $\lambda_{\pm}^{-1}$, we have $\Sigma_{\pm 1}$ in the series of $\lambda_{\pm}^{-1}$. The first approximation of $\Sigma_{\pm 1}$ is enough to obtain (2.20). The convergence of $\Sigma_{\pm 1}$ is, as seen above, uniform for $x\in[x_0, \mp\infty)$,$x_0\in\mathbb{R}$. The estimate and the asymptotic expansion for $\phi_{\pm 2}$ is similarly shown and we omit the calculations. Q.E.D.

The similarity transformation from $\Phi_{\pm}{}^{(0)}$to $\Phi_{\pm}$ plays an important role in both the direct and inverse spectral problems and is defined by

$$\Phi_{\pm}(x) = \Phi_{\pm}{}^{(0)}(x) \mp \int_{\pm\infty}^{x} K_{\pm}(x,y)\Phi_{\pm}{}^{(0)}(y)dy. \tag{2.22}$$

The existence of $K_{\pm}(x,\cdot)$ in $L_2[x, \pm\infty)$ is suggested by the estimate given in Lemma 2. The condition of $Q(x)$ for the existence of $K_{\pm}$, however, is stronger than those given there and presented in the following;

Lemma 3: For $\tilde{Q}_{\pm}\in CF_{\pm}(1)\cap CF'_{\pm}(0)$, $K_{\pm}(x,y)(x\gtrless y)$ exists and has the estimate

$$|K_{\pm}(x,y)| < \tilde{M}_{\pm}(x+y) + I_{\pm}\left(\frac{x+y}{2}\right)\tilde{N}_{\pm}(x), \tag{2.23}$$

$$\tilde{M}_{\pm}(x+y) = \frac{1}{2}\begin{pmatrix}Q_M I_{\pm}\left(\dfrac{x+y}{2}\right) & I'_{\pm}\left(\dfrac{x+y}{2}\right)\\ I'_{\pm}\left(\dfrac{x+y}{2}\right) & Q_M I_{\pm}\left(\dfrac{x+y}{2}\right)\end{pmatrix},$$

where $\tilde{M}_{\pm}(x)$ and $\tilde{N}_{\pm}(x)$ are the matrices with the components, positive and monotonically decreasing as $x\to\pm\infty$, and $I_{\pm}(x)$ is defined by (2.9).

Since $I_{\pm}(x)\subset CF_{\pm}(0)$, the properties $K_{\pm}(x,\cdot)\in L_1[x, \pm\infty)$ and $K_{\pm}(x,\cdot)\in L_2[x, \pm\infty)$ are the direct consequences of (2.23).

Proof. We first assume the existence of $K_{\pm}(x,y)(x\lesseqgtr y)$. The substitution of (2.22) into (2.4) results in the integral equations for

$$M_{\pm}(\xi,\eta) = \begin{pmatrix}K_{\pm 11}(x,y)\\ K_{\pm 22}(x,y)\end{pmatrix}, \quad N_{\pm}(\xi,\eta) = \begin{pmatrix}K_{\pm 12}(x,y)\\ K_{\pm 21}(x,y)\end{pmatrix},$$

where $K_{\pm ij}$ are i,j components of $K_{\pm}$ and $\xi = x+y, \eta = x-y$ $(\eta\lesseqgtr 0)$:

where $K_{\pm ij}$ are i,j components of $K_\pm$ and $\xi = x + y, \eta = x - y$ ($\eta \lesseqgtr 0$):

$$M_\pm(\xi,\eta) = -\frac{1}{2}\int_{\pm\infty}^{\xi} \begin{pmatrix} r_\pm & -q\left(\frac{\xi+\eta}{2}\right) \\ -r\left(\frac{\xi+\eta}{2}\right) & q_\pm \end{pmatrix} N_\pm(\zeta,\eta)d\zeta, \tag{2.24}$$

$$N_\pm(\xi,\eta) = N_\pm(\xi,0) - \frac{1}{4}\int_0^\eta d\zeta \int_{\pm\infty}^{\xi} P_\pm(\xi+\zeta,\nu+\zeta)N_\pm(\nu,\zeta)d\nu, \tag{2.25}$$

where

$$N_\pm(\xi,0) = \mp\frac{1}{2}\begin{pmatrix} \tilde{q}_\pm(\xi/2) \\ \tilde{r}_\pm(\xi/2) \end{pmatrix}, \tag{2.26}$$

$$\begin{aligned} P_\pm(\xi,\eta) &= \begin{pmatrix} q_\pm & q(\xi/2) \\ r(\xi/2) & r_\pm \end{pmatrix}\begin{pmatrix} r_\pm & -q(\eta/2) \\ -r(\eta/2) & q_\pm \end{pmatrix} \\ &= \begin{pmatrix} -q_\pm\tilde{r}_\pm(\eta/2) - \tilde{q}_\pm(\xi/2)r(\eta/2) & q_\pm(q(\xi/2) - q(\eta/2)) \\ r_\pm(r(\xi/2) - r(\eta/2)) & -r_\pm\tilde{q}_\pm(\eta/2) - \tilde{r}_\pm(\xi/2)q(\eta/2) \end{pmatrix}. \end{aligned} \tag{2.27}$$

The Neumann series for $N_\pm(\xi,\eta)$ is obtained from (2.25) as

$$N_\pm(\xi,\eta) = \sum_{m=0}^{\infty} N_\pm^{(m)}(\xi,\eta) \quad (\eta \lesseqgtr 0),$$

$$N_\pm^{(0)}(\xi,\eta) = N_\pm(\xi,0),$$

$$\begin{aligned} N_\pm^{(m)}(\xi,\eta) &= -\frac{1}{4}\int_{\pm\infty}^{\xi} d\xi_1 \int_0^\eta d\eta_1 P_\pm(\xi+\eta_1,\xi_1+\eta_1)N_\pm^{(m-1)}(\xi_1,\eta_1) \\ &= \left(-\frac{1}{4}\right)^m \int_{\pm\infty}^{\xi} d\xi_1 \int_0^\eta d\eta_1 \cdots \int_{\pm\infty}^{\xi_{m-1}} d\xi_m \int_0^{\eta_{m-1}} d\eta_m P_\pm(\xi+\eta_1,\xi_1+\eta_1)\cdots \\ &\quad \times P_\pm(\xi_{m-1}+\eta_m,\xi_m+\eta_m)N(\xi_m,0). \end{aligned}$$

Using the inequality

$$\left|\begin{pmatrix} a & b \\ c & d \end{pmatrix}\begin{pmatrix} a' & b' \\ c' & d' \end{pmatrix}\right| \leqslant \left|\begin{pmatrix} a & b \\ c & d \end{pmatrix}\right| \left|\begin{pmatrix} a' & b' \\ c' & d' \end{pmatrix}\right|,$$

We have from (2.27), under the condition $\xi_{j-1} \lesseqgtr \xi_j$,

$$\begin{aligned} &\left|\int_0^\eta d\eta_j P_\pm(\xi_{j-1}+\eta_j,\xi_j+\eta_j)\right| \leqslant \mp\int_{\pm\infty}^{\eta} d\eta_j |P_\pm(\xi_{j-1}+\eta_j,\xi_j+\eta_j)| \\ &< \mp Q_M \int_{\pm\infty}^{\eta} d\eta_j \begin{pmatrix} \left|\tilde{q}_\pm\left(\frac{\xi_{j-1}+\eta_j}{2}\right)\right| + \left|\tilde{r}_\pm\left(\frac{\xi_j+\eta_j}{2}\right)\right| & \left|q\left(\frac{\xi_{j-1}+\eta_j}{2}\right) - q\left(\frac{\xi_j+\eta_j}{2}\right)\right| \\ \left|r\left(\frac{\xi_{j-1}+\eta_j}{2}\right) - r\left(\frac{\xi_j+\eta_j}{2}\right)\right| & \left|\tilde{r}_\pm\left(\frac{\xi_{j-1}+\eta_j}{2}\right)\right| + \left|\tilde{q}_\pm\left(\frac{\xi_j+\eta_j}{2}\right)\right| \end{pmatrix} \\ &< 2Q_M I_\pm\left(\frac{\xi_{j-1}+\eta}{2}\right)\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \end{aligned}$$

where

$$Q_M = \sup|q| + \sup|r|.$$

Hence,

$$\begin{aligned} |N_\pm^{(m)}(\xi,\eta)| &\leqslant \left(\frac{Q_M}{2}\right)^m \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}^m \left| \int_{\pm\infty}^{\xi} d\xi_1 \cdots \int_{\pm\infty}^{\xi_{m-1}} d\xi_m I_\pm\left(\frac{\xi_1+\eta}{2}\right)\cdots I_\pm\left(\frac{\xi_{m-1}+\eta}{2}\right)|N_\pm(\xi_m,0)| \right| \\ &\leqslant \frac{1}{2(m-1)!}{Q_M}^m I_\pm\left(\frac{\xi+\eta}{2}\right) I_\pm\left(\frac{\xi}{2}\right)\left\{\mp\int_\xi^{\pm\infty} d\zeta\, I_\pm\left(\frac{\zeta+\eta}{2}\right)\right\}^{m-1}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \end{aligned}$$

$$(\eta \lesseqgtr 0, \quad m \geqslant 1)$$

and

$$|N_\pm^{(0)}(\xi,\eta)| \leqslant \tfrac{1}{2} I'_\pm\left(\frac{\xi}{2}\right)\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad I_\pm'(x) = |\tilde{q}_\pm(x)| + |\tilde{r}_\pm(x)|.$$

These estimates and (2.24) lead to the following estimates, which together with (2.24), (2.25), and (2.22) reproduce (2.4);

$$|N_{\pm}(\xi,\eta)|\leqslant\tfrac{1}{2}\left\{I'_{\pm}\left(\frac{\xi}{2}\right)+Q_M I_{\pm}\left(\frac{\xi}{2}\right)I_{\pm}\left(\frac{\xi+\eta}{2}\right)\exp\left[\mp Q_M\int_{\pm\infty}^{\xi}d\zeta\, I_{\pm}\left(\frac{\zeta+\eta}{2}\right)\right]\right\}\begin{pmatrix}1\\1\end{pmatrix},$$

$$|M_{\pm}(\xi,\eta)|\leqslant\frac{Q_M}{2}I_{\pm}\left(\frac{\xi}{2}\right)\left\{1\mp\frac{Q_M}{2}\int_{\pm\infty}^{\xi}d\zeta\, I_{\pm}\left(\frac{\zeta+\eta}{2}\right)\exp\left[\mp Q_M\int_{\pm\infty}^{\xi}d\zeta\, I_{\pm}\left(\frac{\zeta+\eta}{2}\right)\right]\right\}\begin{pmatrix}1\\1\end{pmatrix},$$

or (2.23) with

$$\tilde{M}_{\pm}(x+y)=\frac{1}{2}\begin{pmatrix}Q_M I_{\pm}\left(\frac{x+y}{2}\right), & I_{\pm}'\left(\frac{x+y}{2}\right)\\ I_{\pm}'\left(\frac{x+y}{2}\right), & Q_M I_{\pm}\left(\frac{x+y}{2}\right)\end{pmatrix}$$

and

$$\tilde{N}_{\pm}(x)=\frac{Q_M}{2}\exp\left[\mp Q_M\int_{\pm\infty}^{x}d\zeta\, I_{\pm}\left(\frac{\zeta}{2}\right)\right]\begin{pmatrix}\mp\frac{Q_M}{2}\int_{\pm\infty}^{x}d\zeta\, I_{\pm}\left(\frac{\zeta}{2}\right), & I_{\pm}\left(\frac{x}{2}\right)\\ I_{\pm}\left(\frac{x}{2}\right), & \mp\frac{Q_M}{2}\int_{\pm\infty}^{x}d\zeta\, I_{\pm}\left(\frac{\zeta}{2}\right)\end{pmatrix}.$$

Thus, under the condition given in the lemma, $K_{\pm}(x,y)$ exists and the lemma is proved. Q.E.D.

We consider solution $\tilde{\phi}_{\pm j}$ of (2.1) which has the following asymptotic forms:

$$\tilde{\phi}_{\pm 1}e^{i\lambda_{+}x}=\begin{pmatrix}1\\ \frac{ir_{\pm}}{\lambda+\lambda_{\pm}}\end{pmatrix}+o(1),\quad \nu_{\pm}\gtrless 0$$

$$x\to\pm\infty, \tag{2.28}$$

$$\tilde{\phi}_{\pm 2}e^{-i\lambda_{+}x}=\begin{pmatrix}\frac{-iq_{\pm}}{\lambda+\lambda_{\pm}}\\ 1\end{pmatrix}+o(1),\quad \nu_{\pm}\lessgtr 0$$

where the signs of $\nu_{\pm}$ are opposite to those given in (2.6) for the Jost solutions $\phi_{\pm j}$.

Lemma 4: Let $\tilde{Q}_{\pm}\in CF_{\pm}(0)$ and $\lambda_{\pm}\neq 0$, then (2.1) has the solutions $\tilde{\phi}_{\pm j}$ satisfying the condition (2.28) and ϕ_{+2} and $\tilde{\phi}_{+1}$ (ϕ_{+1} and $\tilde{\phi}_{+2}$) constitute a fundamental system of solutions for $\nu_{+}\geqslant 0$ ($\nu_{+}\leqslant 0$) and similarly ϕ_{-2} and $\tilde{\phi}_{-1}$ (ϕ_{-1} and $\tilde{\phi}_{-2}$) for $\nu_{-}\leqslant 0$ ($\nu_{-}\geqslant 0$).

Proof. It is sufficient to discuss only the case ϕ_{+2} and $\tilde{\phi}_{+1}$ for $\nu_{+}\geqslant 0$. For $\nu_{+}=0$ we put $\tilde{\phi}_{+1}=\phi_{+1}$ which, by (2.6), satisfies (2.28). Since $W[\phi_{+2},\phi_{+1}]\neq 0$, these constitute a fundamental system. For $\nu_{+}>0$ we consider an integral equation

$$\tilde{\phi}_{+1}(x,\lambda,\lambda_{+})=\phi_{+1}^{(0)}(x)+\frac{\lambda+\lambda_{+}}{2\lambda_{+}}\left\{\int_{\infty}^{x}dy\, e^{-i\lambda_{+}(x-y)}\begin{pmatrix}1\\ \frac{ir_{+}}{\lambda+\lambda_{+}}\end{pmatrix}\left(1,\frac{iq_{+}}{\lambda+\lambda_{+}}\right)\tilde{Q}_{+}(y)\tilde{\phi}_{+1}(y)\right.$$

$$\left.+\int_{a}^{x}dy\, e^{i\lambda_{+}(x-y)}\begin{pmatrix}\frac{-iq_{+}}{\lambda+\lambda_{+}}\\ 1\end{pmatrix}\left(\frac{-ir_{+}}{\lambda+\lambda_{+}},1\right)\tilde{Q}_{+}(y)\tilde{\phi}_{+1}(y)\right\} \tag{2.29}$$

which, by $\tilde{\psi}_{+1}=\tilde{\phi}_{+1}e^{i\lambda_{+}x}$, is written as

$$\tilde{\psi}_{+1}(x)=\begin{pmatrix}1\\ \frac{ir_{+}}{\lambda+\lambda_{+}}\end{pmatrix}+\frac{\lambda+\lambda_{+}}{2\lambda_{+}}\left\{\int_{\infty}^{x}dy\begin{pmatrix}1\\ \frac{ir_{+}}{\lambda+\lambda_{+}}\end{pmatrix}\left(1,\frac{iq_{+}}{\lambda+\lambda_{+}}\right)\tilde{Q}_{+}(y)\tilde{\psi}_{+1}(y)\right.$$

$$\left.+\int_{a}^{x}dy\, e^{2i\lambda_{+}(x-y)}\begin{pmatrix}\frac{-iq_{+}}{\lambda+\lambda_{+}}\\ 1\end{pmatrix}\left(\frac{-ir_{+}}{\lambda+\lambda_{+}},1\right)\tilde{Q}_{+}(y)\tilde{\psi}_{+1}(y)\right\}.$$

Let $x\geqslant a$. Since $\tilde{Q}_{+}\in CF_{+}(0)$, we can fix a such that

$$\left|\frac{\lambda+\lambda_{+}}{2\lambda_{+}}\right|\left\{\int_{\infty}^{x}dy\left|\begin{pmatrix}1\\ \frac{ir_{+}}{\lambda+\lambda_{+}}\end{pmatrix}\left(1,\frac{iq_{+}}{\lambda+\lambda_{+}}\right)\tilde{Q}_{+}\right|+\int_{a}^{x}dy\left|\begin{pmatrix}\frac{-iq_{+}}{\lambda+\lambda_{+}}\\ 1\end{pmatrix}\left(\frac{-ir_{+}}{\lambda+\lambda_{+}},1\right)\tilde{Q}_{+}\right|\right\}$$

$$<\left|\frac{\lambda+\lambda_{+}}{2\lambda_{+}}\right|(1+\alpha_{+})^{2}I_{+}(a)=r(a)<1.$$

Then we can determine $\tilde{\psi}_{+1}(x)$ by the successive approximation and have

$$|\tilde{\psi}_{+1}(x)| < \begin{pmatrix}1\\1\end{pmatrix}(1+\alpha_+)\frac{1}{1-r(a)} = r_1(a)\begin{pmatrix}1\\1\end{pmatrix}.$$

Inserting the estimate into the R.H.S. of (2.29) we have for $x\to\infty$

$$\begin{aligned}|(\tilde{\phi}_{+1}-\phi_{+1}^{(0)})e^{i\lambda_+ x}| &< \left|\frac{\lambda+\lambda_+}{2\lambda_+}\right|\left\{\int_x^\infty dy\left|\begin{pmatrix}1\\ \dfrac{ir_+}{\lambda+\lambda_+}\end{pmatrix}\left(1,\frac{iq_+}{\lambda+\lambda_+}\right)\right||\tilde{Q}_+\tilde{\psi}_{+1}|\right.\\ &\quad\left.+\int_a^x dy\, e^{-2\nu_+(x-y)}\left|\begin{pmatrix}\dfrac{-iq_+}{\lambda+\lambda_+}\\ 1\end{pmatrix}\left(\frac{-ir_+}{\lambda+\lambda_+},1\right)\right||\tilde{Q}_+,\tilde{\psi}_{+1}|\right\}\\ &< \left|\frac{\lambda+\lambda_+}{2\lambda_+}\right|(1+\alpha_+)^2 r_1\left\{\int_{x/2}^\infty dy|\tilde{Q}_+| + e^{-\nu_+ x}\int_a^{x/2} dy|\tilde{Q}_+|\right\}\begin{pmatrix}1\\1\end{pmatrix}\\ &< \left|\frac{\lambda+\lambda_+}{2\lambda_+}\right|(1+\alpha_+)^2 r_1\left\{I_+\left(\frac{x}{2}\right)+e^{-\nu_+ x}I_+(a)\right\}\begin{pmatrix}1\\1\end{pmatrix}\to 0,\end{aligned}$$

hence (2.28). It is easy to extend the solution $\tilde{\psi}_{+1}$ or $\tilde{\phi}_{+1}$ given for $x\geqslant a$ to all $x\in\mathbb{R}$. Since $W[\phi_{+2},\tilde{\phi}_{+1}] = -2\lambda_+/(\lambda+\lambda_+)\neq 0$, ϕ_{+2} and $\tilde{\phi}_{+1}$ constitute a fundamental system. Q.E.D.

3. GREEN FUNCTION AND EXPANSION THEOREMS

Let us consider the spectral problem of the operator L of (2.1) in the space $H = L^2(\mathbb{R})\otimes L^2(\mathbb{R})$ constructed from the column vector functions $v(x) = (v_1(x),v_2(x))^T$ with $v_j(x)\in L^2(\mathbb{R})(j=1,2)$. The domain of L, $D(L)\subset H$, contains $v(x)\in H$ such that $v_j(x)$ is absolutely continuous and $Lv\in H$. The resolvent operator $G_\lambda = (L-\lambda)^{-1}$ plays an important role, for the spectrum analysis of L. We study the representation of G_λ as an integral operator on $H = L^2(\mathbb{R})\otimes L^2(\mathbb{R})$ and introduce the Green function $G_\lambda(x,y)$ as the kernel of G_λ. Since our complex plane R_I, the first sheet of the Riemann surface, is divided into four regions R_1–R_4, G_λ also is composed of four functions of λ defined on $\lambda\in R_j (i=1,\cdots,4)$. As discussed in Sec. 2 and exhibited in Fig. 1, the structure of R_1–R_4 depend on the values of $u_\pm$. However, the procedure to obtain the Green function and the expansion theorem does not essentially depend on the values of $u_\pm$. Hence, it may be enough to classify the totality of $u_\pm$ into two groups C_s and C_d and to examine one example from each group: C_s; $u_+^2 - u_-^2\in\mathbb{C}-\mathbb{R}$, C_d; $u_+^2 - u_-^2\in\mathbb{R}$. The group C_s will lead to the expansion theorem with simple continuous spectrum, while C_d to the doubly degenerate spectrum. Below we consider the case $0<|u_-|<|u_+|, 0<\arg u_+<\arg u_-<\pi/2$ as given by Fig. 1 for the group C_s and case $\mathrm{Re}\,u_-<\mathrm{Re}\,u_+$ for the group C_d.

Let us introduce the matrix S, the components of which are defined by the Wronskians of the Jost solutions $\phi_{\pm 1}$ and $\phi_{\pm 2}$,

$$\begin{aligned}\tilde{S}_{11} &= W[\phi_{-1},\phi_{+2}],\quad \tilde{S}_{12} = W[\phi_{-2},\phi_{+2}],\\ \tilde{S}_{21} &= W[\phi_{+1},\phi_{-1}],\quad \tilde{S}_{22} = W[\phi_{+1},\phi_{-2}],\end{aligned}\tag{3.1}$$

where $W[a,b] = a_1b_2 - a_2b_1$ is the Wronskian for the vectors $a = (a_1,a_2)^T$ and $b = (b_1,b_2)^T$. Each of $\tilde{S}_{ij}$ is an analytic function of λ in the region of R_I, if two vector Jost function determining $\tilde{S}_{ij}$ are both analytic there. From the definition of $R_j (1\leqslant j\leqslant 4)$ in R_I, Lemmas 1 and 2, the following lemma is obvious.

Lemma 5: Let $\tilde{Q}_\pm\in CF_\pm(0)$, then for the case C_s

ϕ_{-1}, ϕ_{+2}, $\tilde{S}_{11}$ are analytic for $\lambda\in R_1$,

ϕ_{-1}, ϕ_{+1}, $\tilde{S}_{21}$ are analytic for $\lambda\in R_2$,

ϕ_{-2}, ϕ_{+2}, $\tilde{S}_{12}$ are analytic for $\lambda\in R_3$,

ϕ_{-2}, ϕ_{+1}, $\tilde{S}_{22}$ are analytic for $\lambda\in R_4$,

and for the case C_d the regions R_2 and R_3 disappear.

Thus we derive the asymptotic form of $\tilde{S}_{ij}$ easily from (2.20) and (3.1).

Lemma 6: Let $\tilde{Q}_\pm\in CF(0)_\pm\cap CF'_\pm(0)$. Then the asymptotic form of $\tilde{S}_{ij}$ as $|\lambda|\to\infty$ is given to the order λ^{-1} as follows, in the case C_s;

$$\begin{aligned}\tilde{S}_{11} &= 1 - \frac{1}{2i\lambda}[\pi_-(0)-\pi_+(0)] + o(|\lambda|^{-1}) \quad (\lambda\in R_1),\\ \tilde{S}_{21} &= \frac{1}{2i\lambda}\left(\sum_{x_j>0}\delta r_j e^{-2i\lambda_+ x_j} + \sum_{x_j<0}\delta r_j e^{-2i\lambda_- x_j}\right)\\ &\quad + o(|\lambda|^{-1}), \qquad (\lambda\in R_2),\\ \tilde{S}_{12} &= -\frac{1}{2i\lambda}\left(\sum_{x_j<0}\delta q_j e^{2i\lambda_- x_j} + \sum_{x_j>0}\delta q_j e^{2i\lambda_- x_j}\right)\\ &\quad + o(|\lambda|^{-1}), \qquad (\lambda\in R_3),\\ \tilde{S}_{22} &= 1 + \frac{1}{2i\lambda}[\pi_-(0)-\pi_+(0)] + o(|\lambda|^{-1}), \quad (\lambda\in R_4).\end{aligned}\tag{3.2}$$

In the case C_d the analytic regions R_2, R_3 of $\tilde{S}_{21}$, $\tilde{S}_{12}$ disappear.

From this lemma, it is seen that zeroes of $\tilde{S}_{11}$ and $\tilde{S}_{22}$ are restricted within the bounded regions in R_1 and R_4, respectively. For the later discussion, we introduce two classes of the potentials Q^ϵ and Q^s: Q^ϵ is the subclass of $\tilde{Q}_\pm\in CF_\pm(0)\cap CF'_\pm(0)$ such that the leaps of $Q,\delta Q$ satisfy

$$|\Sigma\delta Q_j e^{i\xi x_j}| > \epsilon\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad (\mathbb{R}\ni\xi\to\infty),\tag{3.3}$$

where ϵ is a positive constant, while Q^s is the subclass of $\tilde{Q}_\pm\in CF_\pm(1)\cap CF_\pm'(0)$, for which $\tilde{S}_{ij}$ has only a finite num-

ber of simple zeros within its analytic region (R_1–R_4) and does not vanish on the boundary of the corresponding region except $\lambda = \infty$. It is noted that for $\tilde{Q}_{\pm} \in Q^e$ the zeros of $\tilde{S}_{21}$ and $\tilde{S}_{12}$ are restricted within the bounded region of R_2 and R_3, respectively, where $\nu_{\pm} \to 0$ as $|\lambda| \to \infty$. A simple example of $\tilde{Q}_{\pm} \in Q^e \cap Q^s$ is the "step potential" $Q(x) = Q_{\pm} (\neq 0) (x \gtrless 0)$.

Let us introduce a function $G_\lambda(x,y)$ by the following formula and prove in Lemma 8 that $G_\lambda(x,y)$ is the Green function for (2.1): For the case C_s, $G_\lambda(x,y) =$

$$
\begin{array}{ll}
x<y & x>y \\
\dfrac{i}{\tilde{S}_{11}}\phi_{-1}(x)\phi_{+2}(y)^A, & \dfrac{i}{\tilde{S}_{11}}\phi_{+2}(x)\phi_{-1}(y)^A, \quad (\lambda \in R_1), \\
-\dfrac{i}{\tilde{S}_{21}}\phi_{-1}(x)\phi_{+1}(y)^A, & -\dfrac{i}{\tilde{S}_{21}}\phi_{+1}(x)\phi_{-1}(y)^A, \quad (\lambda \in R_2), \\
\dfrac{i}{\tilde{S}_{12}}\phi_{-2}(x)\phi_{+2}(y)^A, & \dfrac{i}{\tilde{S}_{12}}\phi_{+2}(x)\phi_{-2}(y)^A, \quad (\lambda \in R_3), \\
-\dfrac{i}{\tilde{S}_{22}}\phi_{-2}(x)\phi_{+1}(y)^A, & -\dfrac{i}{\tilde{S}_{22}}\phi_{+1}(x)\phi_{-2}(y)^A, \quad (\lambda \in R_4),
\end{array}
\tag{3.4}
$$

where v^A is the row vector (v_2, v_1) adjoint to the column vector $v = (v_1, v_2)^T$ and uv^A is the tensor product. For the case C_d, where R_2 and R_3 disappear, $G_\lambda(x,y)$ is composed of two sets of functions defined for $\lambda \in R_1$ and R_4. Further, we introduce some symbols; the set of all zeroes of S_{ij} on the domain of definition R_1–R_4 including its boundary is denoted as $\sigma_p(L)$ and the loci on the λ plane corresponding to its real axes of the $\lambda_{\pm}$ plane (i.e., the curves C_1–C_4 in Fig. 1) as $\sigma_c(L)$ and let $\sigma(L) = \sigma_p(L) + \sigma_c(L)$, $\rho(L) = \mathbb{C} - \sigma(L)$. The analysis in this section will show below that $\sigma_p(L)$, $\sigma_c(L)$, $\sigma(L)$, and $\rho(L)$ are the point spectrum, the continuous spectrum, the spectrum, and the resolvent set of the operator L, respectively.

We present the lemma which plays an important role in the derivation of the expansion theorems. Before it, we must give an estimate of $\phi_{\pm j}(x) (j = 1,2)$ for $x \lesseqgtr 0$.

Lemma 7: For $Q_{\pm} \in CF_{\pm}(0)$, there is a constant $K(\lambda)$ such that

$$
\begin{Bmatrix} |\phi_{\pm 1}(x)| \\ |\phi_{\pm 2}(x)| \end{Bmatrix} < K(\lambda) \begin{pmatrix} 1 \\ 1 \end{pmatrix} \begin{Bmatrix} e^{\nu_+ x} \\ e^{-\nu_+ x} \end{Bmatrix}, \quad \begin{Bmatrix} \nu_{\pm} \lesseqgtr 0 \\ \nu_+ \gtrless 0 \end{Bmatrix}, \quad x \gtrless 0,
$$

$$
\begin{Bmatrix} |\phi_{\pm 1}(x)| \\ |\phi_{\pm 2}(x)| \end{Bmatrix} < K(\lambda) \begin{pmatrix} 1 \\ 1 \end{pmatrix} \begin{Bmatrix} e^{\nu_+ x} \\ e^{-\nu_+ x} \end{Bmatrix}, \quad \begin{Bmatrix} \nu_{\mp} \lesseqgtr 0 \\ \nu_{\mp} \gtrless 0 \end{Bmatrix}, \quad x \lesseqgtr 0.
$$

Proof: The first inequality is the straightforward consequence of Lemma 1 since $I_{\pm}(x)$ is bounded for $x \gtrless 0$. $K(\lambda)$ is a constant larger than $(1 + \alpha_{\pm}) e^{\beta_{\pm} I_{\pm}(0)}$ and determined below. To obtain the second inequality, we expand $\phi_{\pm i}(x)$ for $x \lesseqgtr 0$ by $\phi_{\mp k}, \tilde{\phi}_{\mp i} (i \neq k)$. The expansion coefficients depend on λ but are finite for $\lambda_{\pm} \neq 0$ due to Lemma 4. Then, from the first inequality and (2.28), we have the second. The constant $K(\lambda)$ stands for the maximum of the coefficients of the right hand side of the above four estimates. Q.E.D.

Lemma 8: Let $\tilde{Q}_{\pm} \in CF_{\pm}(0)$, then $G_\lambda (\lambda \in \rho(L))$ is the resolvent operator in H: For $\lambda \in \rho(L)$,

$$
\begin{aligned}
&G_\lambda (L - \lambda) = I, \quad \text{on } D(L) = \text{range of } G_\lambda, \\
&(L - \lambda) G_\lambda = I, \quad \text{on } H.
\end{aligned}
\tag{3.5}
$$

Moreover, G_λ defined by (3.4) separately in $R_1 \sim R_4$ yields a single analytic function with regard to the operator norm in H for $\lambda \in \rho(L) \subset \mathbb{C}$.

Proof: From Lemma 7, we deduce the estimate

$$
|G_\lambda(x,y)| < K(\lambda)^2 \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} e^{-\chi|x-y|}, \quad \lambda \in \rho(L),
$$

where $\chi = \min(|\nu_+|, |\nu_-|)$. Then, for $v \in H$, we have

$$
\begin{aligned}
||G_\lambda v||^2 &\leqslant 2K^4 \int dx \left[\int dy e^{-\chi|y-x|} (|v_1(y)| + |v_2(y)|) \right]^2 \\
&\leqslant 2K^4 \int dx \left(\int dy e^{-\chi|y-x|} \right) \\
&\quad \times \left[\int dy\, e^{-\chi|y-x|} (|v_1(y)| + |v_2(y)|)^2 \right] \\
&\leqslant \frac{8K^4}{\chi} \int dx \int dy\, e^{-\chi|y-x|} (|v_1(y)|^2 + |v_2(y)|^2) \\
&\leqslant \frac{16K^4}{\chi^2} ||v||^2, \quad \text{i.e., } ||G_\lambda|| \leqslant \frac{4K^2}{\chi}, \quad \lambda \in \rho(L).
\end{aligned}
$$

The standard method for the Green function of the differential operator leads to (3.5). Note that L is closable since G_λ is closed. To prove the analyticity of G_λ for $\lambda \in \rho(L)$, it suffices to show that $G_\lambda(x,y)$ for each fixed (x,y) is analytically continuable across the boundaries of $R_j (j = 1$–$4)$. As an example, we consider the case presented by Fig. 1, where the boundary of R_1 and R_2, say, is composed of Λ_+ and C_1. Across Λ_+, $\lambda_-(\lambda)$ is continuous while $\lambda_+(\lambda)$ changes the sign and, hence, $\phi_{+1}(x, \lambda', \lambda_+(\lambda')) \to \phi_{+1}(x, \lambda, -\lambda_+(\lambda))$ and $\phi_{+2}(x, \lambda', \lambda_+(\lambda')) \to \phi_{+2}(x, \lambda, -\lambda_+(\lambda))$ as $R_2 \ni \lambda' \to \lambda$, where $\lambda \in \Lambda_+$ is approached from R_1. Since $\phi_{+1}(x, \lambda, -\lambda_+(\lambda))$ and $\phi_{+2}(x, \lambda, \lambda_+(\lambda))$ are the solutions of (2.1) for the common $\lambda \in \Lambda_+$, they differ only by a factor $C(\lambda)$ determined from the asymptotic forms of ϕ_{+1} and ϕ_{+2},

$$
\phi_{+2}(x, \lambda, -\lambda_+) \to \begin{pmatrix} \dfrac{-iq_+}{\lambda - \lambda_+} \\ 1 \end{pmatrix} e^{-i\lambda x}, \quad x \to \infty,
$$

$$
\phi_{+1}(x, \lambda, \lambda_+) \to \begin{pmatrix} 1 \\ \dfrac{ir_+}{\lambda + \lambda_+} \end{pmatrix} e^{-i\lambda x}, \quad x \to \infty,
$$

for $\lambda \in \Lambda_+ (\nu_+ > 0)$. Thus, we have

$$
\begin{aligned}
&\phi_{+2}(x, \lambda, \lambda_+) = C(\lambda) \phi_{+1}(x, \lambda, -\lambda_+), \quad (\lambda \in \Lambda_+), \\
&C(\lambda) = \frac{-iq_+}{\lambda - \lambda_+} = + \frac{\lambda + \lambda_+}{ir_+},
\end{aligned}
\tag{3.6}
$$

which yields for $\lambda \in \Lambda_+$

$$
\tilde{S}_{11} = W[\phi_{-1}, \phi_{+2}] = -C(\lambda) W[\phi_{+1}, \phi_{-1}] = -C(\lambda) \tilde{S}_{21}.
\tag{3.7}
$$

Substituting (3.6) and (3.7) into $G_\lambda(x,y)$ for $\lambda \in R_1 (x < y)$ in (3.4) and continuing it into R_2 across Λ_+, we see that

$$\frac{1}{\tilde{S}_{11}}\phi_{-1}(x,\lambda,\lambda_-(\lambda))\phi_{+2}{}^{A}(y,\lambda,\lambda_+(\lambda)) \quad (\lambda\in R_1)$$

$$\to -\frac{1}{\tilde{S}_{21}}\phi_{-1}(x,\lambda,\lambda_-(\lambda))\phi_{+1}{}^{A}(y,\lambda,\lambda_+(\lambda)) \quad (\lambda\in R_2).$$

Thus, each $G_\lambda(x,y)$ defined separately on R_1 or R_2 is the analytic continuation of the other. There is no essential difference for the other cases and components. Q.E.D.

From Lemma 8 we obtain easily the identity on $D(L)$,

$$1/\lambda + G_\lambda = (1/\lambda)G_\lambda L, \quad \lambda\in\rho(L). \tag{3.8}$$

We note that (3.8) contains $\lambda_\pm(\lambda)$ only though the Green function which is, by Lemma 8, analytic across the branch cut on the first Riemann sheet R_1 and, for the discussion of (3.8) we may consider the single λ plane without the branch cut, instead of R_1. Let C_ρ be the circle on the λ plane with the center at $\lambda=0$ and the radius ρ sufficiently large and let $w(x)=(w_1(x),w_2(x))^T\in C_0^2(\mathbb{R})$ be the column vector with w_j vanishing outside the finite interval and possessing the continuous second derivative.

Lemma 9: Let $\tilde{Q}_\pm\in Q^e$ and consider the case C_s. Then for $u=Lw$, $w\in C_0^2(\mathbb{R})$

$$\int_{-\infty}^{\infty} dy\, G_\lambda(x,y)u(y) = \begin{cases} O(|\lambda|^{-1}), & |\lambda|\to\infty,\ \lambda\in R_1,R_4 \\ O(1), & |\lambda|\to\infty,\ \lambda\in R_2,R_3, \end{cases} \tag{3.9}$$

$$\int_{C_\rho}\frac{d\lambda}{\lambda}\int_{-\infty}^{\infty} dy\, G_\lambda(x,y)u(y) = O(\rho^{-1}), \quad \rho\to\infty, \tag{3.10}$$

the convergence being uniform in any finite interval of x. For the case $C_d(u_+{}^2-u_-{}^2\in\mathbb{R})$ the first equation of (3.9) and (3.10) hold under the weaker condition $\tilde{Q}_\pm\in CF_\pm(0)\cap CF'_\pm(0)$.

Proof. First, let us show the first equation of (3.9) under the condition $\tilde{Q}_\pm\in Q^e$. In the expression (3.4) in R_1,R_4 we use the asymptotic forms of $\phi_{\pm j}$ given by (2.20);

$$\phi_{\pm 1}-\begin{pmatrix}1\\0\end{pmatrix}e^{-i\lambda_\pm x}, \quad \phi_{\pm 2}-\begin{pmatrix}0\\1\end{pmatrix}e^{i\lambda_\pm x}=O(|\lambda|^{-1}).$$

The contributions to (3.9) by the relevant term of $\phi_{\pm 1},\phi_{\pm 2}$, i.e.,

$$\begin{pmatrix}1\\0\end{pmatrix}e^{-i\lambda_\pm x}, \qquad \begin{pmatrix}0\\1\end{pmatrix}e^{i\lambda_\pm x}$$

are estimated as $O(|\lambda|^{-1})$ through integration by parts. Using (3.2) for $\tilde{S}_{11},\tilde{S}_{22}$ we obtain the first equation. The calculation is similar for the second equation of (3.9) under the condition $\tilde{Q}_\pm\in Q^e$. Under the last condition we consider the special configuration of $\{q_\pm,r_\pm\}\in C_s$ given as Fig. 1. Dividing the λ integral of (3.10) into four parts

$$\int_{C_\rho}\cdot\, d\lambda = \sum_{j=1}^{4}\int_{C_{\rho j}}\cdot\, d\lambda \quad (C_{\rho j}\subset R_j).$$

We derive easily from (3.9)

$$\int_{C_{\rho 1}+C_{\rho 4}}\frac{d\lambda}{\lambda}\int dy\, G_\lambda(x,y)u(y)=O(\rho^{-1}),$$

$$\rho\to\infty, \tag{3.11}$$

$$\int_{C_{\rho 2}+C_{\rho 3}}\frac{d\lambda}{\lambda}\int dy\, G_\lambda(x,y)u(y)=O(\rho^{-1}),$$

since the lengths of the paths in R_2 and R_3 are $O(\rho^{-1})$ and hence we have (3.10). For the case C_d the regions R_2 and R_3 disappear and we obtain the result under the weaker condition. Q.E.D.

Remark. If $p_\pm,s_\pm\neq 0$ for the potential Q in (1.2), the spectrum $\sigma_c(L)$ for $|\lambda|\to\infty$ suffers an important alteration due to the change in (2.3) and the spectral problem requires a separate study.

We exhibit the expansion theorems for the cases C_s and C_d separately.

Theorem 1. Let $\tilde{Q}_\pm\in Q^e\cap Q^s$ and consider the case $C_s(u_+{}^2-u_-{}^2\notin\mathbb{R})$, then we have for $w\in C_0^2(R)$, uniformly in any finite interval of x,

$$w(x)=\lim_{\rho\to\infty}\int_{-\infty}^{\infty} dy\, \Delta_\rho(x,y)w(y), \tag{3.12}$$

$$\Delta_\rho(x,y)=\Delta_\rho{}^{c}(x,y)+\Delta_\rho{}^{d}(x,y),$$

$$\begin{aligned}\Delta_\rho{}^{c}(x,y)=\frac{1}{2\pi}\Bigg\{&-\int_{\vec{C}_{1\rho}}d\lambda\frac{d_+}{\tilde{S}_{11}\tilde{S}_{21}}\phi_{-1}(x)\phi_{-1}{}^{A}(y)\\&-\Bigg\{\int_{\vec{C}_{2\rho}}d\lambda\frac{d_-}{\tilde{S}_{21}\tilde{S}_{22}}\phi_{+1}(x)\phi_{+1}{}^{A}(y)\\&+\int_{\vec{C}_{3\rho}}d\lambda\frac{d_-}{\tilde{S}_{11}\tilde{S}_{12}}\phi_{+2}(x)\phi_{+2}{}^{A}(y)\Bigg\}\Bigg\}\\&+\int_{\vec{C}_{4\rho}}d\lambda\frac{d_+}{\tilde{S}_{12}\tilde{S}_{22}}\phi_{-2}(x)\phi_{-2}{}^{A}(y)\Bigg\},\end{aligned} \tag{3.13}$$

$$\begin{aligned}\Delta_\rho{}^{d}(x,y)=\Bigg\{&-i\sum_{\lambda_k\in R_1}\frac{1}{\tilde{S}_{11}'(\lambda_k)}\phi_{-1}(x)\phi_{+2}{}^{A}(y)\\&+i\sum_{\lambda_k\in R_2}\frac{1}{\tilde{S}_{21}'(\lambda_k)}\phi_{-1}(x)\phi_{+1}{}^{A}(y)\\&-i\sum_{\lambda_k\in R_3}\frac{1}{\tilde{S}_{12}'(\lambda_k)}\phi_{-2}(x)\phi_{+2}{}^{A}(y)\\&+i\sum_{\lambda_k\in R_4}\frac{1}{\tilde{S}_{22}'(\lambda_k)}\phi_{-2}(x)\phi_{+1}{}^{A}(y)\Bigg\},\end{aligned}$$

$$d_\pm=\det T_\pm=2\lambda_\pm/(\lambda+\lambda_\pm),$$

where $\vec{C}_{j\rho}(\overleftarrow{C}_{j\rho})$ denotes the integration to the direction of the arrow along the curve C_j within the circle C_ρ (see Fig. 2 corresponding to Fig. 1) and $\tilde{S}_{ij}'(\lambda_k)$ is the derivative of $\tilde{S}_{ij}$ with respect to λ at $\lambda=\lambda_k$.

Theorem 2: Let $\tilde{Q}_\pm\in Q^s$ and consider the case $C_d(u_+{}^2-u_-{}^2\in\mathbb{R})$, then we have for $w\in C_0^2(\mathbb{R})$ the expansion formula similar to (3.12); if $\arg u_- > \arg u_+$,

$$\begin{aligned}&\Delta_\rho{}^{c}(x,y)=\\&\frac{1}{2\pi}\int_{\vec{C}_{1\rho}+\vec{C}_{4\rho}}d\lambda\left\{\frac{\phi_{-1}(x)\phi_{+2}{}^{A}(y)}{\tilde{S}_{11}}+\frac{\phi_{-2}(x)\phi_{+1}{}^{A}(y)}{\tilde{S}_{22}}\right\}\end{aligned} \tag{3.14}$$

$$+\frac{1}{2\pi}\int_{\vec{C}_5+\vec{C}_6}d\lambda\frac{d_-}{\tilde{S}_{11}\tilde{S}_{22}}\phi_{+2}(x)\phi_{+1}{}^{A}(y),$$

$\Delta_\rho{}^{d}$ having no contribution from R_2 and R_3. Here the integral path $C_{1\rho},(C_{4\rho})$ is obtained as overlap of $C_{1\rho}$ and $C_{2\rho}$ ($C_{3\rho}$ and $C_{4\rho}$) of the preceding theorem, while C_5 and C_6 are nonoverlapping parts (see Fig. 3).

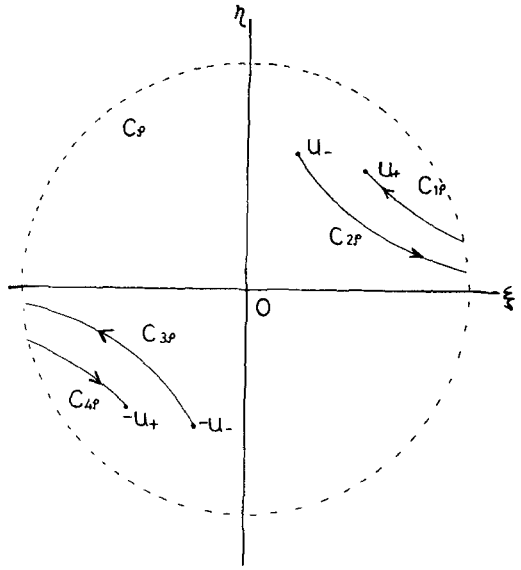

FIG. 2. Curves for the nondegenerate spectrum.

Proof: By (3.8) and (3.10)

$$-2\pi i w(x) = \oint_{C_\rho} d\lambda \int dy\, G_\lambda(x,y) w(y) + O(\rho^{-1}) \quad \text{as } \rho \to \infty \tag{3.15}$$

uniformly in any finite interval of x. We evaluate the first term on the right hand side of (3.15) by modifying C_ρ to the contours along $C_{1\rho}$–$C_{4\rho}$ and $\sigma_\rho(L)$ which, by the assumption, consists of finite number of simple zeroes of $\tilde{S}_{ij}(\lambda)$ and does not overlap to C_j. The integral along the $C_{i\rho}$'s are rearranged by the use of the identities:

$$\phi_{-1}(x,\lambda,\lambda_-) = (1/d_+)(\phi_{+1}(x,\lambda,\lambda_+)\tilde{S}_{11} + \phi_{+2}(x,\lambda,\lambda_+)\tilde{S}_{21}) \quad \text{for } \lambda \in C_1 \quad (\lambda_+ > 0), \tag{3.16a}$$

$$\phi_{-2}(x,\lambda,\lambda_-) = (1/d_+)(\phi_{+1}(x,\lambda,\lambda_+)\tilde{S}_{12} + \phi_{+2}(x,\lambda,\lambda_-)\tilde{S}_{22}) \quad \text{for } \lambda \in C_4 \quad (\lambda_+ < 0), \tag{3.16b}$$

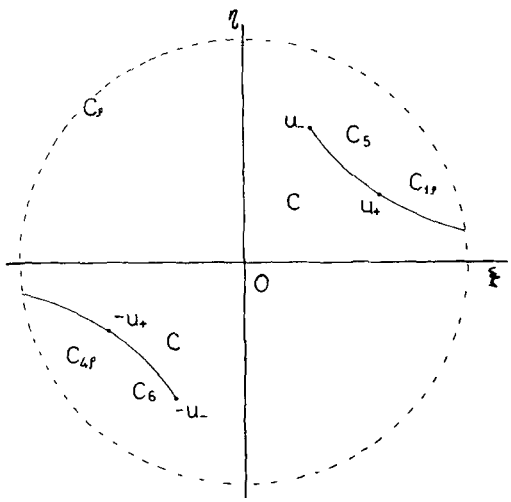

FIG. 3. Curves for the degenerate spectrum.

$$\phi_{+1}(x,\lambda,\lambda_+) = (1/d_-)(\phi_{-1}(x,\lambda,\lambda_-)\tilde{S}_{22} - \phi_{-2}(x,\lambda,\lambda_-)\tilde{S}_{21}) \quad \text{for } \lambda \in C_2 \quad (\lambda_- > 0), \tag{3.16c}$$

$$\phi_{+2}(x,\lambda,\lambda_+) = (1/d_-)(-\phi_{-}(x,\lambda,\lambda_-)\tilde{S}_{12} + \phi_{-2}(x,\lambda,\lambda_-)\tilde{S}_{11}) \quad \text{for } \lambda \in C_3 \quad (\lambda_- < 0), \tag{3.16d}$$

we obtain easily (3.12) and (3.13). For the case C_d, (3.14) is derived analogously. Q.E.D.

In Theorem 1 all the point and continuous spectra, $\sigma_p(L)$ and $\sigma_c(L)$ are simple, while in Theorem 2 some parts of the continuous spectrum are doubly degenerate. From Theorems 1 and 2 we see easily that the continuous spectrum is determined in terms of the asymptotic values $Q_\pm$, while the point spectrum requires the separate examination.

Corollary: The continuous spectra given in Theorems 1 and 2 are stable under the perturbation ΔQ of the potential Q such that $\tilde{Q}_\pm$, $(\tilde{Q}+\Delta Q)_\pm \in Q^c \cap Q^s$ with $\Delta Q_\pm = 0$.

4. SPECTRAL RESOLUTION IN $L^2 \otimes L^2$ AND THE SCATTERING THEORY

We show that the operator L in the Hilbert space $H = ((L^2(\mathbb{R})) \otimes (L^2(\mathbb{R}))$ is a spectral operator in the sense discussed by Dunford and Schwarz, i.e., it has the family of the spectral projection

$\{E(e)\}$ for each bounded set $e \subset \sigma(L) = \sigma_p(L) + \sigma_c(L)$,

under the condition for the potential

$$\tilde{Q}_\pm \in Q^s \cap CF'_\pm(1), \quad u_\pm \neq 0, \quad u_+^2 - u_-^2 \in \mathbb{R}.$$

The last condition indicates that the system belongs to the case C_d defined in the preceding section. We present the Dunford–Schwarz condition for the spectral operator in a convenient form for our application.

Lemma 10 (*Dunford–Schwarz*): Let the closed operator S in the Hilbert space H have a spectrum $\sigma(S)$ which is the disjoint union of a finite set of points $\sigma_p(S) = \{\lambda_1, \cdots, \lambda_n\}$ and of a set $\sigma_c(S)$ contained in a simple Jordan curve C, dividing the complex plane $\mathbb{C}$ into two regions $\mathbb{C}_\pm$. C is expressed by a single valued function $\lambda(t)$ ($t \in \mathbb{R}$), which is smooth, differentiable, and such that the limits $\lambda'(+\infty) = \lambda'(-\infty)$ exist. Suppose that there exists a dense linear manifold $D_0 \subset H$ with the following properties.

(i) For $f,g \in D_0$ there is a constant $K(f,g)$ such that

$$|\lambda|\,|\langle f, R_\lambda g\rangle| < K(f,g), \quad \lambda \in \rho(S) - U(\sigma_p(S)), \tag{4.1}$$

where $R_\lambda = (S-\lambda)^{-1}$ is the resolvent of S, $\langle,\rangle$ denotes the inner product of H, and $U(\sigma_p(S))$ is a neighborhood of $\sigma_p(S)$ in $\mathbb{C}$.

(ii) For each $f,g \in D_0$, $\langle f, R_\lambda g\rangle$ has finite limiting values $R^{\pm}(\hat{\lambda}, f, g)$ as λ approaches almost any point $\hat{\lambda} \in C$ from $\mathbb{C}_\pm$ in a nontangential direction.

(iii) There is a constant M depending only on S such that

$$\int_{\sigma_c(S)} |R^+(\lambda,f,g) - R^-(\lambda,f,g)|\,|d\lambda| \leq M\,\|f\|\cdot\|g\|, \quad f,g \in D_0, \tag{4.2}$$

where $|d\lambda|$ is the arc length along C.

Then S is a spectral operator. For each bounded set $e\subseteq\sigma_c(S)$, the spectral projection $E(e)$ is given by the formula

$$\langle f,E(e)g\rangle = \frac{1}{2\pi i}\int_e \{R^+(\lambda,f,g) - R^-(\lambda,f,g)\}\,d\lambda. \quad (4.3)$$

We obtain the following result for the operator L.

Theorem 3: Let $\tilde{Q}_\pm \in Q^s \cap CF'_\pm(1)$, $u_+^2 - u_-^2 \in \mathbb{R}$, $u_+^2, u_0^2 \neq 0$. Then L in $H = \otimes (L^2(\mathbb{R}))^2$ is a closed operator with $D(L) = D(L_0), L_0 = i\sigma_3\partial/\partial x$ and is a spectral operator in the sense of the preceding lemma.

Proof: We give the proof of the case $u_0^2 = u_+^2 - u_-^2 > 0$ $(u_0 > 0), \pi/2 > \arg u_- > \arg u_+ > 0$ (Fig. 4). In Fig. 4, the curves C_1, C_4, C_5, and C_6 are loci of the continuous spectrum $\sigma_c(L)$ of L. The curves $C_5 + C_1$ and $C_6 + C_4$ are given by functions $\lambda = \lambda^{(\pm)}(t)$, respectively, where

$$\lambda^{(+)}(t) = [(t-1)^2 + u_-^2]^{1/2} \quad (t \geqslant 1)$$
$$\lambda^{(-)}(t) = [(t+1)^2 + u_-^2]^{1/2} \quad (t \leqslant -1).$$

Providing a curve $\lambda^{(0)}(t)$ for $-1 \leqslant t \leqslant 1$ connected to C_5 and C_6 smoothly, we have the curve C of Lemma 10 dividing the complex plane into R_1 and R_2. Under the assumption $\tilde{Q}_\pm \in CF'_\pm(0)$, $|Q(x)|$ is bounded and $Q(x)$ constitutes a bounded operator as a multiplication operator in H. Since it is known that the differential operator L_0 is definable as a closed operator with its domain $D(L_0)$ dense in H, L also is a closed operator with $D(L) = D(L_0)$. We show that the conditions (i)–(iii) of Lemma 10 are satisfied for our resolvent $(L-\lambda)^{-1}$ with the integral kernel $G_\lambda(x,y)$ and with $D_0 = C_0^1$.

(i) Let $f,g \in C_0^1$, $I[f,g] = \mathrm{supp}(f) \cup \mathrm{supp}(g)$ and λ_0 be a constant with the sufficiently large $|\lambda_0|$, then for $x \in I[f,g]$ and $\lambda \in R_1$ with $|\lambda| > |\lambda_0|$, we have, from (2.18) and the asymptotic properties of $\alpha_\pm, \beta_\pm$, and $\gamma_\pm$,

$$\left|\phi_{\pm 1} - \begin{pmatrix}1\\0\end{pmatrix} e^{i\lambda_\pm x}\right| \leqslant \frac{1}{|\lambda_\pm|} K_0 e^{\nu_\pm x}\begin{pmatrix}1\\1\end{pmatrix}, \quad (\nu_\pm \leqslant 0), \quad (4.4a)$$

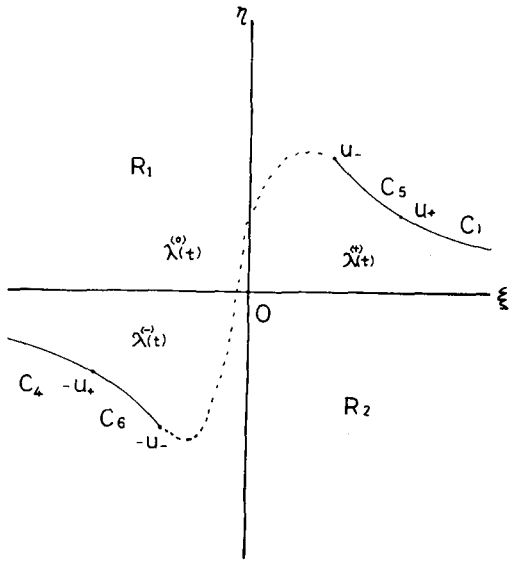

FIG. 4. Jordan curve for the case C_d.

$$\left|\phi_{\pm 2} - \begin{pmatrix}0\\1\end{pmatrix} e^{i\lambda_\pm x}\right| \leqslant \frac{1}{|\lambda_\pm|} K_0 e^{-\nu_\pm x}\begin{pmatrix}1\\1\end{pmatrix}, \quad (\nu_\pm \geqslant 0), \quad (4.4b)$$

where K_0 is a constant independent of x and λ. By virtue of these inequalities and the subsitution of identities

$$\begin{aligned}\phi_{+2}(x)\phi_{-1}(y)^A &= \left[\phi_{+2}(x) - \begin{pmatrix}0\\1\end{pmatrix} e^{i\lambda_\pm x}\right]\left[\phi_{-1}(y) - \begin{pmatrix}1\\0\end{pmatrix} e^{-i\lambda_\pm y}\right]^A \\ &+ \begin{pmatrix}0\\1\end{pmatrix} e^{i\lambda_\pm x}\left[\phi_{-1}(y) - \begin{pmatrix}1\\0\end{pmatrix} e^{-i\lambda_\pm y}\right]^A \\ &+ \left[\phi_{+2}(x) - \begin{pmatrix}0\\1\end{pmatrix} e^{i\lambda_\pm x}\right]\begin{pmatrix}1\\0\end{pmatrix}^A e^{-i\lambda_\pm y} \\ &+ \begin{pmatrix}0 & 0\\1 & 0\end{pmatrix} e^{i\lambda_\pm (x-y)}, \quad (\lambda \in R_1),\end{aligned}$$

and a similar one for $\phi_{-1}(x)\phi_{+2}(y)^A$ into (3.4), it is easy to see that the first term of $\langle f, G_\lambda g\rangle$ for $\lambda \in R_1$ is bounded by $K_1|\lambda|^{-2}$ while the second and the third terms are bounded by $K_2|\lambda|^{-1}$, where K_1 and K_2 are constants, $x,y \in I[f,g]$ and $|\lambda| > |\lambda_0|$. The estimate of the last term is obtained in the form $K_3|\lambda|^{-1}$ through the integration by parts since $f,g \in C_0^1(\mathbb{R})$. Thus, all together, we have $|\langle f, G_\lambda g\rangle| < K|\lambda|^{-1}$ for $|\lambda| > |\lambda_0|$ and a constant K. Since, by Lemma 1 for $\tilde{Q}_\pm \in CF_\pm(1)$, G_λ is continuous in x,y and $\lambda \in R_1$ except at $\lambda \in \sigma_p(L)$, the above discussion implies that $\langle f, G_\lambda g\rangle$ is bounded by $K|\lambda|^{-1}$ for $\lambda \in R_1$ except in the neighborhood of $\sigma_p(L)$. The proof for $\lambda \in R_2$ is similar and we have (4.1).

(ii) for $\tilde{Q}_\pm \in Q^s$, $G_\lambda(x,y)$ is analytic within R_1 and R_2 except at $\lambda \in \sigma_p(L)$ and has continuous boundary values $G_\lambda{}^+(x,y)$ and $G_\lambda{}^-(x,y)$, respectively, on $\sigma_c(L)$ ($\lambda_\pm = 0$ included). Thus, we have

$$\lim_{\epsilon \downarrow 0}\langle f, G_{\lambda \pm i\epsilon\mu} g\rangle = \langle f, G_\lambda{}^\pm g\rangle$$

for $f,g \in C_0^1$ and $\lambda \in \sigma_c$, where $\mu = d\lambda/dt$ specifies the tangential direction along σ_c.

(iii) Due to Theorem 2,

$$G_\lambda{}^c(x,y) \equiv G_\lambda{}^+(x,y) - G_\lambda{}^-(x,y)$$
$$= \begin{cases} \dfrac{1}{2\pi}\left(\dfrac{\phi_{-1}(x)\phi_{+2}{}^A(y)}{\tilde{S}_{11}} + \dfrac{\phi_{-2}(x)\phi_{+1}{}^A(y)}{\tilde{S}_{22}}\right) \\ \qquad\qquad \text{for } \lambda \in C_1 \cup C_4, \\ \dfrac{1}{2\pi}\dfrac{d_-}{\tilde{S}_{11}\tilde{S}_{22}}\phi_{+2}(x)\phi_{+1}{}^A(y) \end{cases}$$

where by (3.16)

$$\begin{aligned}\phi_{-1} &= \frac{1}{d_+}(\phi_{+1}\tilde{S}_{11} + \phi_{+2}\tilde{S}_{21}), \\ &\qquad\qquad \text{for } \lambda \in C_1 \cup C_4, \\ \phi_{-2} &= \frac{1}{d_+}(\phi_{+1}\tilde{S}_{12} + \phi_{+2}\tilde{S}_{22}) \\ \phi_{+1} &= \frac{1}{d_-}(\phi_{-1}\tilde{S}_{22} - \phi_{-2}\tilde{S}_{21}), \\ &\qquad\qquad \text{for } \lambda \in \sigma_c, \\ \phi_{+2} &= \frac{1}{d_-}(-\phi_{-1}\tilde{S}_{12} + \phi_{-2}\tilde{S}_{11}).\end{aligned} \quad (4.5)$$

Since $\phi_{\pm 1}(x),\phi_{\pm 2}(x)$ have the bounded boundary conditions $\sim e^{\pm i\lambda_+ x}$ as $x\to\pm\infty$ for $\lambda\in\sigma_c$ and, for $\tilde{Q}_\pm\in CF_\pm(1)$, are continuous in x and λ by Lemma 1, they are bounded for $x\in[0,\pm\infty),\lambda\in\sigma_c$. Hence under the assumption $\tilde{Q}_\pm\in Q^s$, $\tilde{S}_{ij}(\lambda),(i,j=1,2)$, $\tilde{S}_{11}^{-1}$ and $\tilde{S}_{22}^{-1}$ are bounded for $\lambda\in\sigma_c$.

First let $\lambda\in C_5$ or C_6, then we can express G_λ^c in terms of these bounded functions;

$$G_\lambda{}^c(x,y)=\begin{cases}\dfrac{1}{2\pi}\dfrac{d_-}{\tilde{S}_{11}\tilde{S}_{22}}\phi_{+2}(x)\phi_{+1}{}^A(y), & x,y\geqslant 0,\\ \dfrac{1}{2\pi}\dfrac{1}{\tilde{S}_{11}}\phi_{+2}(x)\left\{\phi_{-1}(y)-\dfrac{\tilde{S}_{21}}{\tilde{S}_{22}}\phi_{-2}(y)\right\}^A, & x\geqslant 0,y\leqslant 0,\\ \dfrac{1}{2\pi}\dfrac{1}{\tilde{S}_{22}}\left\{-\dfrac{\tilde{S}_{12}}{\tilde{S}_{11}}\phi_{-1}(x)+\phi_{-2}(x)\right\}\phi_{+1}{}^A(y), & x\leqslant 0,y\geqslant 0,\\ \dfrac{1}{2\pi}\dfrac{1}{d_-}\left\{-\dfrac{\tilde{S}_{12}}{\tilde{S}_{11}}\phi_{-1}(x)+\phi_{-2}(x)\right\}\\ \quad\times\left\{\phi_{-1}(y)-\dfrac{\tilde{S}_{12}}{\tilde{S}_{22}}\phi_{-2}(y)\right\}^A, & x,y\leqslant 0.\end{cases}$$

Thus, $G_\lambda{}^c(x,y)$ is bounded except in the last equation which has the factor $d_-{}^{-1}\propto\lambda_-{}^{-1}$. Since, however, $\lambda\neq 0$ on C_5 and C_6, the change of the variable from λ to λ_- implies that the integral

$$I_{5+6}=\int_{C_5+C_6}|d\lambda\,|\,|\langle f,G_\lambda{}^c g\rangle|=\int_{-u_0}^{u_0}|d\lambda_-|\left|\frac{\lambda_-}{\lambda}\right|\langle f,G_\lambda{}^c g\rangle$$

exists for all expressions of $G_\lambda{}^c$ and we have

$$I_{5+6}\leqslant M_1\langle|f|,|g|\rangle\leqslant M_1\|f\|\cdot\|g\|, \tag{4.6}$$

where M_1 is a constant depending on u_0.

For $\lambda\in C_1$ or C_4, we introduce a large constant ρ such that C_1 and C_4 are divided into two parts as

$$C_{1\rho}:1\leqslant t\leqslant t_\rho,\quad 0\leqslant\lambda_+\leqslant\lambda_{+\rho},\quad|\lambda|\leqslant\rho,$$
$$C_{1\infty}:t_\rho\leqslant t,\quad\lambda_{+\rho}\leqslant\lambda_+,\quad|\lambda|\geqslant\rho,$$
$$C_{4\rho}:-t_\rho\leqslant t\leqslant -1,\quad-\lambda_{+\rho}\leqslant\lambda_+\leqslant 0,\quad|\lambda|\leqslant\rho,$$
$$C_{4\infty}:t\leqslant -t_\rho,\quad\lambda_+\leqslant-\lambda_{+\rho},\quad|\lambda|\geqslant\rho.$$

We have analogously as I_{5+6}

$$\begin{aligned}I_{1\rho+4\rho}&=\int_{C_{1\rho}+C_{4\rho}}|d\lambda\,\|\langle f,G_\lambda{}^c g\rangle|\\&=\int_{-\lambda_{+\rho}}^{\lambda_{+\rho}}d\lambda_+\left|\frac{\lambda_+}{\lambda}\right||\langle f,G_\lambda{}^c g\rangle|\leqslant M_2\|f\|\cdot\|g\|,\end{aligned} \tag{4.7}$$

where $\lambda=(\lambda_+{}^2+u_+{}^2)^{1/2}\neq 0$ on $C_{1\rho},C_{4\rho}$ by $u_+{}^2\neq 0$. Finally we estimate

$$\begin{aligned}I_{1\infty+4\infty}&=\int_{C_{1\infty}+C_{4\infty}}|d\lambda\,\|\langle f,G_\lambda{}^c g\rangle|\\&=\frac{1}{2\pi}\int|d\lambda\,|\left|\frac{1}{\tilde{S}_{11}}\int dx\,\bar{f}^T\phi_{-1}\int dx\,\phi_{+2}{}^A g+\frac{1}{\tilde{S}_{22}}\right.\\&\quad\left.\times\int dx\,\bar{f}^T\phi_{-2}\int dx\,\phi_{+1}{}^A g\right|,\quad|t|>t_\rho\end{aligned} \tag{4.8}$$

where, for example, by (4.5)

$$\int dx\,\bar{f}^T\phi_{-1}=\int_{-\infty}^0 dx\,\bar{f}^T\phi_{-1}+\frac{\tilde{S}_{11}}{d_+}\int_0^\infty dx\,\bar{f}^T\phi_{+1}+\frac{\tilde{S}_{21}}{d_+}\int_0^\infty dx\,\bar{f}^T\phi_{+2}.$$

Due to Lemma 2 and asymptotic properties of $\alpha_\pm,\beta_\pm$, and $\gamma_\pm$ for large $|\lambda|\,(\lambda\in C_{1\infty}\cup C_{4\infty})$, we have

$$\begin{aligned}&\left|\int_{-\infty}^0 dx\,\bar{f}^T\phi_{-1}\right|\\&\quad<\left|\int_{-\infty}^0 dx\left(\bar{f}_1+\frac{ir_-}{\lambda+\lambda_-}\bar{f}_2\right)e^{-i\lambda x}\right|\\&\quad+\frac{1}{|\lambda_+|}M_2\int_{-\infty}^0 dx(|f_1|+|f_2|)(J_-(x)+\alpha_-{}^2|\lambda_-|I_-(x))\end{aligned} \tag{4.9}$$

with M_2 a constant. The first term of the right hand side of (4.9) is the Fourier transform of the function of $C_0(\mathbb{R})$ and hence square integrable with respect to λ_-. The second term is bounded, as verified by the Schwarz inequality, by

$$\frac{1}{|\lambda_+|}M_3\int_{-\infty}^0 dx[\,J_-(x)+\alpha_-{}^2|\lambda_-|I_-(x)]\cdot\|f\|,$$

where M_3 is a constant depending on $J_-(0),I_-(0)$ and ρ, and the integrations of $J_-(x)$ and $I_-(x)$ in x exist for $\tilde{Q}_\pm\in CF_\pm(1)\cap CF_\pm'(1)$. Collecting these inequalities together, we obtain $\int_{|t|>t_\rho}|d\lambda\,\|\int_{-\infty}^0 dx\,\bar{f}^T\phi_{-1}|^2$ $<\text{constant}\times\|f\|^2$. Other integrals in (4.8) can be treated similarly and we have the inequality

$$I_{1\infty+4\infty}<M\|f\|\cdot\|g\|, \tag{4.10}$$

where M depends on t_ρ and $\tilde{Q}_\pm$ but not on f and g. The equations (4.6), (4.7), and (4.10) yield (4.2) for our operator L. Q.E.D.

In the above theorem, we restrict ourselves to the case of $u_\pm\neq 0$ and C_d. If, for instance, $u_+=0$ and u_- is pure imaginary, σ_c crosses with itself at $\lambda=0$ and does not constitute a simple Jordan curve as assumed in Lemma 10. The spectral problem for the later case, as well as the case C_s, will be studied in the future.

Finally, we summarize the relation of the Jost solutions $\Phi_\pm$ on $\sigma_c(L)$ [see (3.16a)–(3.16d)] and briefly consider the scattering problem

$$\left.\begin{aligned}\phi_{+1}+\frac{\tilde{S}_{21}}{\tilde{S}_{11}}\phi_{+2}&=\frac{d_+}{\tilde{S}_{11}}\phi_{-1},\\ \phi_{+2}+\frac{\tilde{S}_{12}}{\tilde{S}_{22}}\phi_{+1}&=\frac{d_+}{\tilde{S}_{22}}\phi_{-2},\end{aligned}\right\}\lambda_+(\lambda)\in\mathbb{R}, \tag{4.11a, 4.11b}$$

$$\left.\begin{aligned}\phi_{-1}-\frac{\tilde{S}_{21}}{\tilde{S}_{22}}\phi_{-2}&=\frac{d_-}{\tilde{S}_{22}}\phi_{+1},\\ \phi_{-2}-\frac{\tilde{S}_{12}}{\tilde{S}_{11}}\phi_{-1}&=\frac{d_-}{\tilde{S}_{11}}\phi_{+2}.\end{aligned}\right\}\lambda_-(\lambda)\in\mathbb{R}. \tag{4.11c, 4.11d}$$

First we consider the special configuration $u_+{}^2-u_-{}^2>0$ (case C_d). For the degenerate continuous spectrum $\lambda\in C_1+C_4(\lambda_\pm\in\mathbb{R})$, (4.11a) describes the scattering of a plane wave incident at $x=+\infty,\phi_{+1}{}^{(0)}$ by the potential $\tilde{Q}_+$ with a reflected plane wave $(\tilde{S}_{21}/\tilde{S}_{11})\phi_{+2}{}^{(0)}$ at $x=+\infty$ and

a transmitted plane wave $(d_+/\tilde{S}_{11})\phi_{-1}^{(0)}$ at $x = -\infty$ and similarly for (4.11b)–(4.11d). Thus we may define the reflection coefficients $r_{+1} = \tilde{S}_{21}/\tilde{S}_{11}$, $r_{+2} = \tilde{S}_{12}/\tilde{S}_{22}$, $r_{-1} = -\tilde{S}_{21}/\tilde{S}_{22}$, $r_{-2} = -\tilde{S}_{12}/\tilde{S}_{11}$ and the transmission coefficients $t_{+1} = d_+/\tilde{S}_{11}$, $t_{+2} = d_+/\tilde{S}_{22}$, $t_{-1} = d_-/\tilde{S}_{22}$, $t_{-2} = d_-/\tilde{S}_{11}$ for $\lambda \in C_1 + C_4$. For the simple continuous spectrum $\lambda \in C_5 + C_6 (\lambda_- \in \mathbb{R}, \lambda_+ \notin \mathbb{R}$, see Fig. 4), we have the relations $\tilde{S}_{11}\tilde{S}_{22} = \tilde{S}_{21}\tilde{S}_{12}$ and $\tilde{S}_{12}/\tilde{S}_{22} = -ir_+/(\lambda + \lambda_+)$ and (4.11c) is equivalent to (4.11d), whereas (4.11a) and (4.11b) do not hold. In this case the incident plane wave $\phi_{-1}^{(0)}$ at $x = -\infty$ is accompanied by a reflected plane wave $\phi_{-2}^{(0)}$ but no transmitted plane wave at $x = +\infty$. In the configuration $u_+^2 - u_-^2 \notin \mathbb{R}$ (case C_s), only one of two Jost solutions $\phi_{+1,2}$ and $\phi_{-1,2}$ is bounded for $\lambda_- \in \mathbb{R}, x = +\infty$ and $\lambda_+ \in \mathbb{R}, x = -\infty$, respectively. Hence one equation from (4.11a) and (4.11b) for $\lambda_+ \in \mathbb{R}$ and one from (4.11c) and (4.11d) for $\lambda_- \in \mathbb{R}$ may be used to describe the reflection of a plane wave at $x = +\infty$ and $-\infty$ without a transmitted plane wave at $x = -\infty$ and $+\infty$, respectively. The scattering theory for the cases C_d and C_s in terms of the similarity transformation $K_\pm$ of Sec. 2 will be discussed elsewhere.

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Sensitivity theory for nonlinear systems. I. Nonlinear functional analysis approach [a)]

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(Received 14 April 1981; accepted for publication 22 June 1981)

Concepts of nonlinear functional analysis are employed to investigate the mathematical foundations underlying sensitivity theory. This makes it possible not only to ascertain the limitations inherent in existing analytical approaches to sensitivity analysis, but also to rigorously formulate a considerably more general sensitivity theory for physical problems characterized by systems of nonlinear equations and by nonlinear functionals as responses. Two alternative formalisms, labeled the "forward sensitivity formalism" and the "adjoint sensitivity formalism," are developed in order to evaluate the sensitivity of the response to variations in the system parameters. The forward sensitivity formalism is formulated in normed linear spaces, and the existence of the Gâteaux differentials of the operators appearing in the problem is shown to be both necessary and sufficient for its validity. This formalism is conceptually straightforward and can be advantageously used to assess the effects of relatively few parameter alterations on many responses. On the other hand, for problems involving many parameter alterations or a large data base and comparatively few functional-type responses, the alternative adjoint sensitivity formalism is computationally more economical. However, it is shown that this formalism can be developed only under conditions that are more restrictive than those underlying the validity of the forward sensitivity formalism. In particular, the requirement that operators acting on the state vector and on the system parameters must admit densely defined Gâteaux derivatives is shown to be of fundamental importance for the validity of this formalism. The present analysis significantly extends the scope of sensitivity theory and provides a basis for still further generalizations.

PACS numbers: 02.30.Sa

I. INTRODUCTION

The use of adjoint functions for sensitivity analysis appeared as early as the 1940's. The main approaches to sensitivity analysis were either based on perturbation theory or based on variational approaches. In reactor theory, for example, the first use of perturbation theory is attributed[1] to Wigner,[2] while the variational principles are considered[3] to have evolved from works of Levine and Schwinger[4] and Roussopolos.[5] The scope of both the variational formulation and the perturbation theory approach has subsequently been generalized and extended (see, e.g., Refs. 6–12). The great potential of adjoint-function based approaches to sensitivity analysis of several linear problems encountered in reactor theory has been demonstrated in the comprehensive reviews given by Stacey[3] and Greenspan.[12] These successes have generated considerable interest in extending and applying such approaches to sensitivity analysis of several inherently nonlinear problems in other areas.[13–17] Higher-order perturbation theories have also been proposed[18] for sensitivity analysis of neutronics problems involving linear operators. Recent developments, through 1979, in adjoint-operator based approaches to sensitivity and uncertainty analyses have been comprehensively reviewed by Weisbin *et al.*[19]

To date, several alternative theoretical approaches to adjoint-based sensitivity equations have evolved, the three prominent being:

1. variational approaches,[3,7,9,10,14]
2. perturbation theory approaches, including "generalized perturbation theory,"[6,8,12,13,16,18]
3. differential approaches.[15,17]

All of these approaches have been focused on deriving expressions for the sensitivities of the system responses (i.e., system performance parameters) to changes in the input parameters. The system responses considered in these approaches have been particular forms of functionals, and the sensitivities have been defined as the derivatives of these responses with respect to the input parameters. However, the necessary and sufficient conditions underlying the validity of these approaches have not been rigorously analyzed. Consequently, questions have been raised[20] regarding the applicability of these approaches to sensitivity analysis of problems that are more complex than those treated so far; of current practical interest are, for example, thermal-hydraulics problems involving discontinuous state functions and parameters.

In a recent article, Cacuci *et al.*[21] have introduced and employed concepts of nonlinear functional analysis[22–24] in an attempt to set sensitivity theory on a more rigorous mathematical foundation, and to extend the scope of the theory. In addition, they have also presented a sensitivity theory formulation for a class of discretized nonlinear systems, and have enlarged the type of functionals considered as responses. Although, rigorous within explicitly stated limitations, their derivations repeatedly required the existence of the Frechet derivatives[22–26] of the various operators, without providing an analysis of the motivations underlying the *ne-*

[a)]Research sponsored by Electric Power Research Institute (RP 1441-1) under subcontract with Oak Ridge National Laboratory, operated by Union Carbide Corporation for the U. S. Department of Energy.

 0022-2488/81/122794-09$01.00

cessity of these requirements. Since operators that are not Frechet differentiable can also be encountered in practice, an investigation of the aforementioned question of necessity is clearly needed.

In view of the high level of current interest in sensitivity theory, there is a strong incentive to present a detailed investigation of its underlying mathematical aspects. This investigation is carried out by employing the concepts and methods of nonlinear functional analysis.[22-26] As a result, a sensitivity theory is formulated here in a considerably more general framework than before.

The system of nonlinear operator equations and the associated response, a general nonlinear functional, are introduced and described in Sec. II; altogether, they are intended to be sufficiently general to include—as particular cases—the mathematical representation of a large number of problems in a wide variety of fields. The problem is formulated here in normed linear spaces over the scalar field of real numbers. This choice of space is sufficiently general for the purposes of this study:

1. it provides the framework for the clear exposition of the necessary and sufficient conditions underlying the sensitivity theory formalisms presented in Sec. III,

2. it opens the possibility to establish the limitations inherent in the previous approaches (by direct comparison with the present approach),

3. it provides a basis for still further extensions of the theory.

The formulation of the sensitivity theory presented in Sec. III is centered on evaluating the Gâteaux differential[22,24,25] of the response; this quantity is considered to be "the most general measure of the sensitivity of a response to variations in the system parameters."[27] Consequently, Secs. IIIA and IIIB are devoted to the presentation of the two alternative methods for evaluating this Gâteaux differential. The conceptually and computationally straightforward method is labeled the "forward sensitivity formalism," and is dealt with in Sec. IIIA. The alternative method, labeled the "adjoint sensitivity formalism," is presented in Sec. IIIB. The motivation underlying the development of the "adjoint sensitivity formalism" is well known[1-19,21] this formalism is a great deal more economical to apply, *if possible*, to the broad class of practical problems characterized by large data bases and comparatively few responses. However, the present analysis also reveals a fact that does not seem to have been noticed so far: the "adjoint sensitivity formalism" can be formulated *only* under conditions that are more restrictive than those underlying the formulation of the "forward sensitivity formalism."

The limitations inherent in the previous approaches[1-19,21] to sensitivity theory are assessed in Sec. IV by examination of their underlying assumptions and by comparison to the formalisms presented in Sec. III. The results arrived at in this study are then reviewed and summarized in Sec. V. There, the particularly important relationship between the representation of the "indirect effect term" as an inner product, and the construction of the "adjoint sensitivity formalism" is also underscored. By drawing attention to this special relationship, the ground is prepared for an accompanying paper[28] whose objective is to extend sensitivity theory to more complicated responses.

Finally, some thoughts are offered on possible directions for future research aimed at further generalizations of the theory presented here.

II. MATHEMATICAL REPRESENTATION OF THE PHYSICAL PROBLEM

Consider, for the sake of generality, that the physical problem under consideration is represented by the following system of K coupled nonlinear equations written in operator form as

$$\mathbf{N}[u(x),\alpha(x)] = \mathbf{Q}[\alpha(x),x]. \tag{1}$$

The quantities appearing in Eq. (1) are defined as follows:

1. $x = (x_1,...,x_J)$ is the phase-space position vector $x \in \Omega \subset \mathscr{R}^J$, where Ω is a subset of the J-dimensional real vector space $\mathscr{R}^J$,

2. $u(x) = [u_1(x),...,u_K(x)]$ is the state vector; $u(x) \in E_u$, where E_u is a normed linear space over the scalar field Λ of real numbers,

3. $\alpha(x) = [\alpha_1(x),...,\alpha_I(x)]$ is the vector of system parameters; $\alpha \in E_\alpha$, where E_α is also a normed linear space. In practical applications, E_α may be one of the Hilbert spaces L_2 or l_2; occasionally, the components of α may simply be a set of real scalars, in which case E_α is $\mathscr{R}^I$,

4. $\mathbf{Q}[\alpha(x),x] = [Q_1(\alpha,x),...,Q_K(\alpha,x)]^T$ is a (column) vector whose elements represent inhomogeneous source terms (the symbol T denoted "transposition"); $\mathbf{Q} \in E_Q$, where E_Q is again a normed linear space. The components of $\mathbf{Q}$ may be operators (rather than just functions) acting on $\alpha(x)$ and x,

5. the components of the (column) vector $\mathbf{N} = [N_1(u,\alpha),...,N_K(u,\alpha)]^T$ are nonlinear operators acting, in general, not only on the state vector $u(x)$, but also on the vector of system parameters $\alpha(x)$.

In view of the definitions given above, $\mathbf{N}$ represents the mapping $\mathbf{N}: S \subset E \to E_Q$, where $S = S_u \times S_\alpha, S_u \subset E_u, S_\alpha \subset E_\alpha$, and $E = E_u \times E_\alpha$. Note that an arbitrary element $e \in E$ is of the form $e = (u,\alpha)$. Even though in most practical applications E and E_Q will be Hilbert spaces (e.g., the space L_2, the Sobolev spaces H^m), this restriction is not imposed at this stage for the sake of generality. In the same vein of generality, the components of $\mathbf{N}$ are considered here to be defined in terms of operators such as differential, difference, integral, distributions, or infinite matrices. The domain S of $\mathbf{N}$ is, of course, intimately related to the characteristics of these operators. Thus, if differential operators appear in Eq. (1), then a corresponding set of boundary and/or initial conditions—which is essential to define S—must also be given. This set can be represented as

$$\{\mathbf{B}(u,\alpha) - \mathbf{A}(\alpha)\}_{\partial\Omega} = 0, \tag{2}$$

where $\mathbf{A}$ and $\mathbf{B}$ are operators and $\partial\Omega$ is the boundary of Ω; the operator $\mathbf{A}(\alpha)$ represents all inhomogeneous boundary terms.

To be definite, $u(x)$ is considered to be the unique nontrivial solution of the physical problem described in Eqs. (1) and (2). This requirement is usually fulfilled (or assumed to be fulfilled when rigorous existence and uniqueness proofs are lacking) in most problems of practical interest. The fol-

lowing purposes are accomplished as consequences of imposing this requirement:

1. elimination from further consideration of those points in nonlinear problems where bifurcation (i.e., branching) of solutions occurs,

2. inclusion of the treatment of source-free problems as a special case of Eq. (1).

In this vein, Eq. (1) is considered to include any equality constraints that $u(x)$ might be required to satisfy. The specifications introduced so far are sufficiently general to allow Eqs. (1) and (2) to include, as particular cases, the mathematical modeling of a wide range of problems of practical interest in many diverse fields.

The system response (i.e., performance parameter) R associated with the problem modeled by Eqs. (1) and (2) must also be specified. The response considered here is a general nonlinear functional of e, and is represented by the mapping

$$R(e): D \subset E \rightarrow \Lambda, \tag{3}$$

where D is considered to be finitely open[23] at e, and where Λ is the underlying scalar field of real numbers. Equation (3) represents a significant extension over the particular forms of nonlinear functionals considered as responses in previous works.[15,17-19,21]

III. SENSITIVITY THEORY

The most general and fundamental concept for the definition of the sensitivity[27] of a response to variations in the system parameters is the Gâteaux (G) differential. The G differential[29] $VR(e^0;h)$ of $R(e)$ at e^0 with increment h, is defined as[22,24,25,30,31]

$$\lim_{t \to 0} [R(e^0 + th) - R(e^0)]/t = VR(e^0;h) \tag{4}$$

for $t \in \Lambda$, and all (i.e., arbitrary) vectors $h \in E$; here, $h = (h_u, h_\alpha)$, since $E = E_u \times E_\alpha$.

The G differential $VR(e^0;h)$ is related to the total variation[21,30] $[R(e^0 + h) - R(e^0)]$ of R at e^0 through the relationship

$$R(e^0 + h) - R(e^0) = VR(e^0;h) + \Delta(h), \tag{5}$$

where

$$\lim_{t \to 0} [\Delta(th)/t] = 0.$$

It is important to note that, in view of the properties of the G differential, R need not be continuous in u and/or α for $VR(e^0;h)$ to exist at $e^0 = (u^0, \alpha^0)$, and that $VR(e^0;h)$ is not necessarily linear in h. It thus becomes apparent that by defining $VR(e^0;h)$ to be *the sensitivity of the response R*, the definitions of sensitivity encountered in the previously mentioned works[1-19] are considerably generalized and extended. With the present definition, the concept of sensitivity also becomes meaningful for certain types of physical problems and responses which could not have been treated within the framework of the previous approaches.[1-19] The circumstances under which the present definition of sensitivity [i.e., $VR(e^0;h)$] reduces to the previous ones will be discussed in detail in Sec. IV.

Thus, the objective of the sensitivity theory to be presented in this study is to evaluate $VR(e^0;h)$. To achieve this objective, two alternative formalisms—the "forward sensitivity formalism" and the "adjoint sensitivity formalism"—are developed and discussed.

A. The "forward sensitivity formalism"

It is observed that, given the vector of "changes" h_α around the "base-case configuration" α^0, the sensitivity $VR(e^0;h)$ of $R(e)$ at e^0 can be evaluated only after determining the vector h_u, since h_u and h_α are not independent. A relationship between h_u and h_α is obtained by taking the G differentials of Eqs. (1) and (2). This gives

$$V\mathbf{N}(e^0;h) - V\mathbf{Q}(\alpha^0;h_\alpha) = \mathbf{0}, \tag{6}$$

and

$$\{V\mathbf{B}(e^0;h) - V\mathbf{A}(\alpha^0;h_\alpha)\}_{\partial\Omega} = \mathbf{0}, \tag{7}$$

respectively. Of course, the above system of equations—which will subsequently be referred to as the "forward sensitivity equations"—is meaningful if and only if (iff) the respective G differentials of the operators **N**, **B**, **Q**, and **A** exist. Note again that these G differentials need not necessarily be linear operators in either h_u or h_α, and that their existence does not require the operators **N**, **B**, **Q**, and **A** to be continuous in u or α at e^0.

For a given vector of "changes" h_α around α^0, one must be able to solve the system given in Eqs. (6) and (7) to obtain h_u; otherwise, of course, it would be impossible to perform sensitivity analysis of the given physical system. [However, a detailed analysis of the conditions under which Eqs. (6) and (7) can be solved for h_u is not within the scope of this work.] Once h_u is determined, it can be employed, in turn, to evaluate the sensitivity $VR(e^0;h)$ of $R(e)$ at e^0, for a given vector of "changes" h_α.

It should be noted here that the "forward sensitivity formalism" is characterized in a fundamental sense by the fact that the solution h_u of the h_α-dependent "forward sensitivity equations" [viz., Eqs. (6) and (7)] is needed to evaluate $VR(e^0;h)$. Consequently, from the standpoint of computational costs, the "forward sensitivity formalism" is advantageous to employ only if, in the problem under consideration, the number of different responses of interest exceeds the number of input parameters. However, a large number of problems of practical interest are characterized by very large data bases (i.e., α has many components) and comparatively few responses. In such situations, it is not economical to employ the "forward sensitivity formalism" to answer all sensitivity questions that might arise in practice, since it becomes prohibitively expensive to repeatedly solve the h_α-dependent "forward sensitivity equations" to determine h_u for all possible vectors h_α. Hence, it is clearly desirable to devise (if possible) an alternative procedure to evaluate $VR(e^0;h)$, to avoid the necessity of repeatedly solving the "forward sensitivity equations."

B. The "adjoint sensitivity formalism"

The ideas underlying this alternative procedure to evaluate sensitivities were seeded in the earliest works[2,4,5] on sensitivity analysis of reactor physics problems, and they

have remained substantially unchanged. These ideas are recalled now in order to motivate the direction of the nonlinear functional analysis-based derivations to be presented in this section.

In all previous works,[1-19] it was possible to separate the expression giving the sensitivity of the response functional [corresponding to our $VR(e^0;h)$] into two terms: the "direct effect term"—involving only quantities corresponding to our h_α, and the "indirect effect term"—involving only quantities corresponding to our h_u. The "indirect effect term" was subsequently expressed as an inner product involving

1. a function corresponding to our h_u, and

2. a function that ultimately became the source term for the "adjoint equations."

A system of equations formally adjoint to equations corresponding to our "forward sensitivity equations" was introduced, solved and the resulting solution used to evaluate the "indirect effect term." Since the resulting "adjoint equations" were independent of changes in the input parameters, the solution of these equations was computed once and for all per response. In turn, this opened the way to an economical evaluation of the "indirect effect term," for all possible combinations of changes in the input parameters.

The above-mentioned procedure has been employed for a long time to perform sensitivity analysis of the (conceptually simpler) linear problems in reactor physics and shielding,[1-12] and has been formally extended in recent years to certain nonlinear problems.[13-19] However, the derivations underlying this procedure have been carried out in a heuristic manner, and their formal characteristics are underscored by the fact that the necessary and sufficient conditions for their validity have not yet been analyzed rigorously. As already mentioned, sufficient conditions for the applicability of such a procedure to sensitivity analysis of nonlinear problems in real Hilbert spaces have been stated in Ref. 21. There, it was shown that an adjoint operator-based procedure can be rigorously formulated, provided that Fréchet derivatives of the nonlinear operators describing the physical problem [viz., Eqs. (1)–(3)] exist. However, the following analysis will show that such a procedure—can be formulated without requiring the existence of Fréchet derivatives. This procedure will subsequently be referred to as the "adjoint sensitivity formalism."

In view of the foregoing discussion, it becomes clear that the development of this "adjoint sensitivity formalism" must be focussed on constructing an adjoint system that is (i) uniquely defined, (ii) independent of the vectors h_u and h_α, and (iii) such that its solution can be used to eliminate all unknown values of h_u from the expression of $VR(e^0;h)$. Adjoint operators can only be introduced uniquely for densely defined linear operators in Banach spaces. However, at this stage, $V\mathbf{N}(e^0;h)$, $V\mathbf{B}(e^0;h)$, and $VR(e^0;h)$ are not necessarily linear in h, and E is not necessarily complete. It follows that developing the "adjoint sensitivity formalism" requires the introduction of restrictions in addition to those underlying the validity of the "forward sensitivity formalism."

There are several equivalent theorems[22,25] giving necessary and sufficient conditions in order that a nonlinear operator $F(e)$ with domain in E and range in another normed linear space (in particular, E_Q or Λ) admit a G differential $VF(e^0;h)$ at e^0 that is linear in h. A set of such conditions is provided by the following theorem[22]:

Theorem: the G-differential $VF(e^0;h)$ of F at e^0 is linear in $h \in E$ iff:

$F(e)$ satisfies a weak Lipschitz condition at e^0, and:

$$F(e^0 + th_1 + th_2) - F(e^0 + th_1) - F(e^0 + th_2) + F(e^0) = o(t). \tag{8}$$

A G differential $VF(e^0;h)$ that is linear in h is customarily denoted by $DF(e^0;h)$; furthermore, $DF(e^0;h) = F'_e(e^0)h$, where $F'_e(e^0)$ is the G derivative[22,25,31,32] of F at e^0. This shows that, in the present case, $V\mathbf{N}(e^0;h)$ and $V\mathbf{B}(e^0;h)$ are linear in h iff $\mathbf{N}$ and $\mathbf{B}$ satisfy, in turn, conditions identical to those stated in Eq. (8) for $F(e)$.

For the purposes of subsequent derivations, $V\mathbf{N}(e^0;h)$ and $V\mathbf{B}(e^0;h)$ are henceforth considered to be linear in h, and denoted by $D\mathbf{N}(e^0;h)$ and $D\mathbf{B}(e^0;h)$, respectively. Recalling now that, in our case, $E = E_u \times E_\alpha$, it further follows that

$$D\mathbf{N}(e^0;h) = \mathbf{N}'_u(e^0)h_u + \mathbf{N}'_\alpha(e^0)h_\alpha \tag{9}$$

and

$$D\mathbf{B}(e^0;h) = \mathbf{B}'_u(e^0)h_u + \mathbf{B}'_\alpha(e^0)h_\alpha. \tag{10}$$

In the above expressions, $\mathbf{N}'_u(e^0)$ and $\mathbf{B}'_u(e^0)$ denote, respectively, the partial G derivatives[25] at e^0 of $\mathbf{N}$ and $\mathbf{B}$ with respect to u, while $\mathbf{N}'_\alpha(e^0)$ and $\mathbf{B}'_\alpha(e^0)$ denote the partial G derivatives at e^0 of $\mathbf{N}$ and $\mathbf{B}$ with respect to α. Note that $\mathbf{N}'_u(e^0)$ and $\mathbf{B}'_u(e^0)$ are linear operators in h_u with domain in E_u and range in E_Q [i.e., $\mathbf{N}'_u(e^0), \mathbf{B}'_u(e^0) \in \mathscr{L}(E_u, E_Q)$], and are independent of h_α; similarly, $\mathbf{N}'_\alpha(e^0)$, $\mathbf{B}'_\alpha(e^0) \in \mathscr{L}(E_\alpha, E_Q)$, and are independent of h_u. The explicit representation of $\mathbf{N}'_u(e^0)$ and $\mathbf{N}'_\alpha(e^0)$ are matrices whose elements are the partial G derivatives at e^0 of the components of $\mathbf{N}$ with respect to the components of u and the components of α. [The elements of the matrices representing $\mathbf{B}'_u(e^0)$ and $\mathbf{B}'_\alpha(e^0)$ are obtained in a similar manner.] For example, $\mathbf{N}'_u(e^0)$ is represented by the matrix

$$\mathbf{N}'_u(e^0) = [L_{ij}(e^0)]; \quad L_{ij}(e^0) = (N_i)'_{u_j}(e^0); \quad i,j = 1,\ldots,K. \tag{11}$$

In view of Eqs. (9) and (10), the "forward sensitivity equations" [given in Eqs. (6) and (7)] become

$$\mathbf{N}'_u(e^0)h_u = V\mathbf{Q}(\alpha^0;h_\alpha) - \mathbf{N}'_\alpha(e^0)h_\alpha \tag{12}$$

and

$$\{\mathbf{B}'_u(e^0)h_u\}_{\partial\Omega} = \{V\mathbf{A}(\alpha^0;h_\alpha) - \mathbf{B}'_\alpha(e^0)h_\alpha\}_{\partial\Omega}. \tag{13}$$

Although $\mathbf{N}'_u(e^0), \mathbf{B}'_u(e^0) \in \mathscr{L}(E_u, E_Q)$, further progress toward constructing the desired adjoint system can be made only if $\mathbf{N}'_u(e^0)$ is densely defined and the underlying normed linear spaces are complete. (Otherwise, of course, adjoint operators cannot be uniquely determined.) Since the lack of an inner product in a general Banach space gives rise to significant conceptual distinctions between the adjoint of a linear operator on a Banach space and the adjoint of a linear operator on a Hilbert space, the choice of space becomes important for subsequent derivations. To motivate the

choice to be made here, it is recalled that all of the previous approaches to sensitivity theory made use of real inner products. Therefore, clarification of the conditions underlying the validity of these approaches is facilitated by the simplifying properties of Hilbert spaces. Specifically, the spaces E_u and E_Q are henceforth required to be real Hilbert spaces, denoted by H_u and H_Q, respectively. The inner products on H_u and H_Q are denoted by $\langle\ ,\ \rangle$ and $(\ ,\ )$ respectively.

Since Hilbert spaces are self-dual, the following relationship holds for a vector $v \in H_Q$:

$$(v, \mathbf{N}'_u(e^0)h_u) = \langle L^*(e^0)v, h_u\rangle + \{P[h_u, v]\}_{\partial\Omega}. \tag{14}$$

In the above equation, the operator $L^*(e^0)$ is the $K \times K$ matrix

$$L^*(e^0) = [L^*_{ji}(e^0)], \quad i,j = 1,\ldots,K \tag{15}$$

obtained by transposing the formal adjoints of the operators $L_{ij}(e^0)$, and $\{P[h_u, v]\}_{\partial\Omega}$ is the associated bilinear form evaluated on $\partial\Omega$. The domain of L^* is determined by selecting appropriate adjoint boundary conditions, represented here in operator form as

$$\{\mathbf{B}^*(v;e^0) - \mathbf{A}^*(e^0)\}_{\partial\Omega} = \mathbf{0}. \tag{16}$$

These boundary conditions are obtained by requiring that

1. they be independent of h_u, h_α, and G derivatives with respect to α, and

2. the substitution of Eqs. (13) and (16) into the expression of $\{P[h_u, v]\}_{\partial\Omega}$ must cause all terms containing unknown values of h_u to vanish.

This selection of the adjoint boundary conditions reduces $\{P[h_u, v]\}_{\partial\Omega}$ to a quantity designated here by $\hat{P}[h_\alpha, v; e^0]$, where $\hat{P}$ contains boundary terms involving only known values of h_α, v, and (possibly) e^0. In general, $\hat{P}$ does not automatically vanish as a result of these manipulations,[33] although it may do so in particular instances. Hence, Eq. (14) can also be written as

$$(v, \mathbf{N}'_u(e^0)h_u) = \langle L^*(e^0)v, h_u\rangle + \hat{P}[h_\alpha, v; e^0]. \tag{17}$$

The above equation can be further transformed by recalling Eq. (12); then Eq. (17) becomes

$$\langle L^*(e^0)v, h_u\rangle = (v, V\mathbf{Q}(\alpha^0; h_\alpha) - \mathbf{N}'_\alpha(e^0)h_\alpha) - \hat{P}[h_\alpha, v; e^0]. \tag{18}$$

Note that the right-hand side of Eq. (18) does not contain any values of h_u. Thus, if in the functional $VR(e^0;h)$ the h_u dependence could be separated from the h_α dependence, and the quantity containing this h_u dependence could be expressed in terms of the left-hand side of Eq. (18), then the construction of the "adjoint sensitivity formalism" would be concluded. However, $\langle L^*(e^0)v, h_u\rangle$ is linear in h_u, while in general, $VR(e^0;h)$ is not. For $VR(e^0;h)$ to be linear in h (and, consequently, in h_u), it becomes apparent that $R(e)$ must be required to satisfy the same conditions as those required of $F(e)$ in Eq. (8). Then, the linear G differential $VR(e^0;h)$ is denoted by $DR(e^0;h)$, and can be expressed as

$$DR(e^0;h) = R'_u(e^0)h_u + R'_\alpha(e^0)h_\alpha, \tag{19}$$

where $R'_u(e^0)$ and $R'_\alpha(e^0)$ are, respectively, the partial G derivatives at e^0 of $R(e)$ with respect to u and α.

As desired, the h_u dependence has been separated from the h_α dependence. Note here that, historically, quantities corresponding to the functionals $R'_u(e^0)h_u$ and $R'_\alpha(e^0)h_\alpha$ have been referred to as the "indirect effect term" and the "direct effect term," respectively. This terminology reflects the fact that in the previous works[1-19] the response was considered to depend on α both "directly" and "indirectly"—via the state vector u, i.e., the response was considered to be a mapping from the space of the input parameters into the real numbers. Although this interpretation of the response is in contradistinction with the concepts introduced and employed in this work, it is still convenient to continue to use this traditional terminology when referring to $R'_u(e^0)h_u$ and $R'_\alpha(e^0)h_\alpha$.

Since the functional $R'_u(e^0)h_u$ is linear in h_u and since Hilbert spaces are self-dual, the Riesz representation theorem[26] ensures that there exists a unique vector $\nabla_u R(e^0) \in H_u$ such that

$$R'_u(e^0)h_u = \langle \nabla_u R(e^0), h_u\rangle, h_u \in H_u. \tag{20}$$

At this stage, it can be required that the right-hand side of Eq. (20) and the left-hand side of Eq. (18) represent the same functional. Then, the Riesz representation theorem ensures that the relationship

$$L^*(e^0)v = \nabla_u R(e^0) \tag{21}$$

holds uniquely, where v satisfies the boundary conditions given in Eq. (16).

The construction of the desired adjoint system—consisting of Eqs. (21) and (16)—has thus been completed. Furthermore, the desired elimination of the unknown values of h_u from the expression giving the sensitivity $DR(e^0;h)$ of $R(e)$ at e^0 to variations h_α has also been accomplished, since in view of Eqs. (18)–(21),

$$DR(e^0;h) = R'_\alpha(e^0)h_\alpha + (v, V\mathbf{Q}(e^0;h_\alpha) - \mathbf{N}'_\alpha(e^0)h_\alpha) - \hat{P}[h_\alpha, v; e^0]. \tag{22}$$

Once the single calculation to determine the adjoint function v is performed, Eq. (22) provides the most efficient means to obtain the sensitivity $DR(e^0;h)$ of $R(e)$. However, it is important to reemphasize that Eq. (22) holds if and only if all the requirements imposed in this section on the various operators are satisfied.

IV. COMPARATIVE DISCUSSION OF PREVIOUS APPROACHES

In all of the works based on the differential[15,17] and the generalized perturbation theory[3,8,13,16,18,19] approaches to sensitivity analysis, the problems were *a priori* considered to depend explicitly and implicitly through the state functions on the system parameters. [The terminology "generalized perturbation theory" is customarily used in works on reactor theory[3] to denote that the perturbation estimate obtained accounts not only for effects resulting directly from the alteration of the system parameters (i.e., "perturbation theory") but also for indirect effects arising from the changes in the state function (i.e., the dependent variable) due to the system alteration, without explicitly calculating the altered state function.] This would conceptually correspond to interpreting the problem under consideration (including the response) as a complicated mapping of a subset $D_\alpha \subset E_\alpha$ into the set Λ

of real numbers. Consequently, in order to obtain expressions for the sensitivity coefficients, the respective derivations must rely explicitly and/or implicitly on the existence and uniform continuity of the derivatives of the operators and the state functions with respect to the system parameters (and, possibly, with respect to the phase-space variables).

In the works dealing with nonlinear problems, it was further stated that the "differentiated equations"[15,17] (obtained by formally differentiating the nonlinear operator equations and response with respect to an arbitrary input parameter) or, correspondingly, the "equations for the altered state functions"[13,16] (obtained by formal first-order perturbation theory expansions around the "base-case configuration" of the state functions and input parameters) are linear. In fact, these equations correspond conceptually to our "forward sensitivity equations" given in Eqs. (6) and (7). This correspondence makes the conditions underlying the validity of the "differentiated equations" or the "equations for the altered state functions" become evident: as derived,[13,15-17] these equations are rigorously valid only if the input parameters are real scalars, if the derivatives of the various state functions with respect to these input parameters are uniformly continuous, and if all operators (including the response) appearing in the formulation of the problem under consideration admit Fréchet derivatives[22,25] with respect to the state functions. It should also be mentioned that, in these works,[15-17] the adjoint system was always assumed to exist, and was introduced in a heuristic manner with initially unspecified source terms. These source terms were subsequently identified with the "derivatives of the response with respect to the state functions" by making use of inner products. Again, linearity of this "response derivative"[15,17] (or, correspondingly, linearity of the "response perturbation" with respect to the "perturbations in the state functions"[13,16]) was implicitly assumed. Furthermore, the uniqueness of the end products (e.g., adjoint systems, sensitivities) was assumed but not actually demonstrated.

The variational approaches[3,7,10,14] relied on constructing an appropriate variational functional, which was subsequently required to satisfy a stationarity condition for the base-case values of the state functions and system parameters. Expressions for the sensitivity coefficients then resulted from this requirement. In the earlier formulations [see, e.g., Ref. 3, p. 6], an unspecified function appeared in the expression of the variational functional to be made stationary. This function was subsequently identified with the "adjoint" function that satisfied an "adjoint system" whose existence was *a priori* assumed. Significant advances were made (see, e.g., Stacey's review[3]) in modifying earlier variational principles by using Lagrange multipliers so that restrictions which are mathematically necessary to impose on the class of trial functions correspond to the physical conditions associated with the original problem and, just as important, so that the constraints are directly incorporated in the variational principle. Although considerable ingenuity is always required to construct an appropriate variational functional—whose explicit form depends on the problem under consideration—these variational approaches did not require (in principle) the existence of derivatives of the state functions with respect to the system parameters. In this sense, the assumptions underlying these variational approaches are less restrictive than the assumptions underlying the previously mentioned differential and generalized perturbation theory approaches. However, derivatives of the various operators with respect to the state functions and the system parameters were still needed. Although the exact nature of these derivatives (and, consequently, the necessary and sufficient conditions underlying their existence) were not generally analyzed, Stacey defines and employs a quantity referred to in his work[3] as the "variation of a functional." In the light of the concepts of nonlinear functional analysis,[22,25] it becomes apparent that his definition is in fact the definition of the Fréchet differential of that functional. This implies that the "functional derivatives" encountered in these variational approaches[3,14] must be interpreted as Fréchet derivatives.

It is noted that these approaches[1-19] to sensitivity analysis were developed to analyze specific practical problems encountered in reactor physics, shielding, depletion, and heat transfer. These specific problems involved sufficiently well-behaved operators, and the parameters considered for sensitivity analysis were, in fact, real scalars. Therefore, even though the derivation underlying these approaches are mathematically not entirely rigorous, the end results are essentially correct.

In reformulating both the differential and the variational approaches to sensitivity analysis of nonlinear systems of equations, Cacuci *et al.*[21] considered a typical nonlinear problem as a mapping defined on a product space corresponding to $E = E_u \times E_\alpha$ as defined in Sec. II. (Note, however, that these spaces were considered at the outset to be Hilbert spaces.) This completely eliminated the need for the existence of derivatives of the state vector with respect to the system parameters. In addition, the definition of sensitivity of a response was generalized to allow consideration of system parameters that were functions rather than just scalars. By requiring the existence of partial Fréchet derivatives[22,25] of the operators with respect to the state vector and the system parameters, the existence of an appropriate adjoint system was ensured. Although this work generalized and extended the scope of the previously available sensitivity theory formulations, the existence of partial Fréchet derivatives is not actually essential for sensitivity analysis; as shown in Sec. III, the existence of the G differentials—for the "forward sensitivity formalism,"—or of the partial G derivatives with respect to the state vectors only—for the "adjoint sensitivity formalism"—are both necessary and sufficient.

Although the concept of an inner product has been essential to formulating the existing adjoint-function based approaches[1-19,21] to sensitivity analysis, the implications associated with the particular use of this concept in these works have not been generally discussed. Clearly, the prerequisite for employing an inner product is that the problem under consideration must be formulated in an appropriate Hilbert (or at least pre-Hilbert) space. Furthermore, since a single definition for the inner product was used in each of these works when introducing adjoint operators, the underlying implication is that the problem being analyzed can only in-

volve operators with ranges in the same Hilbert space to which the state vector belongs. By contrast, the "adjoint sensitivity formalism" developed here makes use of two distinct inner products [cf., Eq. (14) *et seq.*]; this allows sensitivity analysis of problems involving operators whose ranges may be in a Hilbert space that differs from the Hilbert space to which either the state vector or the system parameters belong. Also, it is noted that no distinctions were made in previous works[1-19,21] regarding the fundamental mathematical differences between the requirements underlying the "forward" formulations and those underlying the "adjoint" formulations of sensitivity theory. The present work provides a basis for assessing the potentially important practical consequences of these differences.

The forgoing discussion has highlighted the major aspects regarding the specific uses of perturbation theory and variational approaches for applications to sensitivity analysis. For such applications, the common scope of these approaches is to obtain sensitivities. In reactor theory, for example, some authors[3,34] regarded perturbation theory as an application of variational methods in the sense that a variational formulation "is employed to derive a generalized perturbation theory for estimating the change in the physical quantity of interest which would take place if the properties of the system were to be altered" (Ref. 3, p. 18). But the general uses of either perturbation theory or variational methods are not limited to deriving sensitivity functions. Similarities as well as distinctions between the perturbation theory and the variational approaches to sensitivity analysis, and the contributions that this work brings to sensitivity theory can be further clarified by briefly analyzing the relationships between perturbation theory, variational methods, and functional analysis from a broader perspective.

Perturbation theory and variational methods are not sharply defined disciplines; they are bodies of knowledge unified more by the respective method of approach than by clear-cut demarcation of their respective provinces. For example, the terminology "perturbation theory" is also encountered in celestial mechanics and in nonlinear oscillation theory. However, although these "perturbation theories" study systems deviating slightly from an ideal system for which the complete solution is known, the problems they treat and the tools they use are quite different from those used to derive sensitivities. In reactor theory, for example,[35] this latter use of perturbation theory has evolved from the work of Rayleigh on vibrating systems and of Schrödinger in quantum mechanics.

The works based on perturbation theory to derive sensitivities for problems involving linear operators tacitly assume that the eigenvalues and eigenvectors admit series expansions in a small parameter that measures the deviation of the "unperturbed operator" from the "unperturbed" one. Without a proof that the series actually converges, it is difficult to decide whether the first term of the series gives an adequate picture introduced by the perturbation, a fact well known in reactor theory,[35] for example. For applications to sensitivity analysis of problems involving linear operators, the underpinnings of the perturbation theory approach lie in linear functional analysis. Although a systematic presentation of perturbation theory for linear operators is now available,[36] further work remains to be done to fully exploit these functional-analytic techniques for sensitivity analysis.

Variational methods, just like perturbation theory, are not developed specifically for sensitivity analysis, although the variational principles developed for this purpose are, of course, very useful. But variational principles, even those restricted to limited classes of variations, are difficult to formulate and for many nonlinear problems of interest (e.g., thermal hydraulics, heat and mass transfer) variational principles are not yet available.[37] Furthermore, a systematic and general treatment of variational principles for problems involving nonlinear operators must necessarily rely on the differential concepts of nonlinear functional analysis, i.e., Gâteaux and Fréchet differentials and derivatives.

The present work attempts to provide a general framework for systematic sensitivity analysis of both linear and nonlinear systems. The scope of the theory formulated here is to derive sensitivities, to be used not only for predicting the behavior of the response when the system parameters are altered, but also for ranking the importance of these parameters, and for performing uncertainty analysis by combining the sensitivities with the appropriate parameter covariances.

The link between a rigorous perturbation theory (and/or variational) approach to sensitivity analysis and the sensitivity theory presented in this work is provided by functional analysis. In particular, the similar overall strategy and the use of adjoint operators stem from functional-analytic concepts. In this sense, the greater general validity and applicability of the present sensitivity theory also contributes to the development of perturbation theory for applications to nonlinear systems. Finally, it is noted that whenever the variational, differential, and perturbation theory approaches are rigorously applicable, the end results for the sensitivities are identical to those produced by the sensitivity theory presented in this work.

V. SUMMARY AND CONCLUSIONS

The methods and concepts of abstract analysis have been employed to formulate a sensitivity theory for physical problems described by systems of coupled nonlinear equations, and nonlinear functionals as responses. Greater generality has been achieved by considering the problem and the response as mappings defined on the product space $E = E_u \times E_\alpha$. Consequently, it has been possible to circumvent the need to assume a specific form for the functional representing the response $R(e)$. The scope and versatility of the present formulation of sensitivity theory have also been extended by defining the sensitivity of the response to variations in the system parameters (α) as the G differential $VR(e^0;h)$ of $R(e)$ at e^0.

Two alternative formalisms have been developed to evaluate the sensitivity $VR(e^0;h)$ of $R(e)$: the "forward sensitivity formalism" and the "adjoint sensitivity formalism." As has been shown, there are clear distinctions between the necessary and sufficient conditions required for the validity of each formalism. On the one hand, it has been demonstrated that the "forward sensitivity formalism" can be rigorous-

ly formulated in normed linear spaces, and that the existence of the G differentials of all operators appearing in the original nonlinear equations are the necessary and sufficient conditions underlying the validity of this formalism. It has also been emphasized that these G differentials are not linear operators.

On the other hand, it has been shown that the necessary and sufficient conditions underlying the validity of the "adjoint sensitivity formalism" are more restrictive. Most prominent among these conditions is the requirement that all operators acting on the state vector u must admit densely defined partial G derivatives at $e^0 = (u^0, \alpha^0)$ with respect to u. Furthermore, the underlying normed linear spaces have to be complete in order that the adjoint sensitivity formalism" be unique and generally valid. By setting the development of this formalism in Hilbert spaces, the Riesz representation theorem[26] was shown to play a fundamental role. Although this theorem does not hold in general in a pre-Hilbert space [e.g., $\nabla_u R(e^0)$ in Eq. (20) may not exist], in many practical applications it may do so. Thus, the "adjoint sensitivity formalism" may still be applicable to certain problems which fit naturally in a pre-Hilbert space that may not be convenient to complete in practice. (Theoretically, of course, pre-Hilbert spaces can always be completed.)

Note that the need to introduce *any* derivatives of operators acting *solely* on the system parameters α, or derivatives of the state vector with respect to α, has been completely eliminated. As has been shown, the existence of the G differentials $V\mathbf{Q}(\alpha^0; h_\alpha)$ and $V\mathbf{A}(\alpha^0; h_\alpha)$ is both necessary and sufficient. Furthermore, the use of two distinct inner products [cf., Eq. (14) *et seq*] makes it possible to treat problems involving operators whose range is not in the same Hilbert space as the state vector. Finally, the results obtained by employing the previous approaches[1-19,21] to sensitivity theory can be recovered as particular forms of the results obtained here. Altogether, these factors contribute to the greater generality and applicability of the "adjoint sensitivity formalism" presented here.

It is of practical interest to mention that, in particular applications, additional conditions may need to be imposed on the operators **N**, **B**, **Q**, and **A**, in order to solve Eqs. (1) and (2) by some particular numerical procedure. For example, several of the most widely used numerical methods[31] for solving nonlinear operator equations require the existence of Fréchet derivatives of **N** and **B** at e^0; in such cases, the conditions underlying the validity of the "adjoint sensitivity formalism" would automatically be satisfied.

The sensitivity theory presented in this study has been restricted to responses that are functionals. This highlighted the intimate connection between the construction of the adjoint system and the mathematical nature of the response. This connection is underscored by recalling the essential role played by the Riesz representation theorem when identifying the sensitivity of the response with an inner product [cf., Eqs. (20) and (22)]. In fact, it would not have been possible to employ the "adjoint sensitivity formalism"—or any of the previously mentioned approaches[1-19,21]—if the response had not been a functional.

Hence, a logical step toward further extensions of sensitivity theory is the consideration of more complicated responses. Results in this direction have been obtained, and will be presented in an accompanying paper.[28]

ACKNOWLEDGMENTS

This work would not have been possible without the strong support of J. Naser of the Electric Power Research Institute and C. R. Weisbin and F. C. Maienschein of Oak Ridge National Laboratory (ORNL) Engineering Physics Division. Stimulating discussions with A. Solomon, J. H. Marable, E. M. Oblow, and M. C. G. Hall of ORNL are gratefully acknowledged. Special thanks are due to Ethel Cagle, Ann Houston and Patti Boit for their expert typing of this paper.

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e^0, reserving the term "differential" for those instances when VR is linear in its second argument h. Others refer to VR as the weak differential of R at e^0, to distinguish it from the strong (or Fréchet) differential of R at e^0. However, the terminology employed in this study appears to occur most frequently in the latest works on nonlinear operators.

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[33]In principle, $\hat{P}$, could have been forced to vanish if appropriate extensions (in the operator sense) of $N'_u(e^0)$ had been considered. Of course, this would have necessitated the reformulation of Eqs. (12) and (13). In practice, however, it is more convenient to avoid such complications, since $\hat{P}$ appears (ultimately) only as a readily computable quantity in the final expression the "indirect effect" term [cf., Eq. (22)].

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Sensitivity theory for nonlinear systems. II. Extensions to additional classes of responses [a)]

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(Received 14 April 1981; accepted for publication 31 July 1981)

This work extends a recent, functional-analytic formulation of sensitivity theory to include treatment of additional types of responses. There are physical systems where a critical point of a function that depends on the system's state vector and parameters defines the location in phase-space where the response functional is evaluated. The Gâteaux differentials giving the sensitivities of both the functional and the critical point to changes in the system's parameters are obtained by alternative formalisms. The foward sensitivity formalism is the simpler and more general, but may be prohibitively expensive for problems with large data bases. The adjoint sensitivity formalism, although less generally applicable and requiring several adjoint calculations, is likely to be the only practical approach. Sensitivity theory is also extended to include treatment of general operators, acting on the system's state vector and parameters, as response. In this case, the forward sensitivity formalism is the same as for functional responses, but the adjoint sensitivity formalism is considerably different. The adjoint sensitivity formalism requires expanding the indirect effect term, an element of a Hilbert space, in terms of elements of an orthonormal basis. Since as many calculations of adjoint functions are required as there are nonzero terms in this expansion, careful consideration of truncating the expansion is needed to assess the advantages of the adjoint sensitivity formalism over the forward sensitivity formalism.

PACS numbers: 02.30.Sa

I. INTRODUCTION

Concepts of nonlinear functional analysis have been employed in an accompanying paper[1] to formulate a rigorous and comprehensive sensitivity theory for physical problems characterized by systems of coupled nonlinear equations. The formulation of this theory is centered on evaluating the Gâteaux (G) differential of the system response (i.e., performance parameter) associated with the physical problem. This G differential is a general and fundamental concept for defining the sensitivity of a response to variations in the system parameters. The nonlinear functional defining the response in Ref. 1 can be used as a general representation for any response that is solely characterized by a numerical value. Note that only this numerical value changes when varying the system parameters.

However, responses which cannot be characterized solely by a numerical value are often encountered in practice. In reactor safety and design, for example, responses of considerable interest are the maximum temperature in the cladding, the maximum power density, and the maximum normalized reactor power level (if point-kinetics equations are used in the transient reactor analysis code). Such responses are characterized both by the numerical value at the maximum and by the position in phase-space where the maximum occurs. In this case, varying the system parameters alters not only the value at this maximum but also alters the position of the maximum in phase-space. This is illustrated in Sec. II, where sensitivity theory is extended to allow treatment of a general response comprising, as particular cases, the representation of maxima, minima, and saddle points. Important practical consequences arising from the conceptual differences between such a response and certain functionals considered as response in previous applications of sensitivity theory are underscored in Sec. IIC. by presenting a comparative analysis of results obtained for a reactor thermal-hydraulics sample problem.

To date, the responses considered in adjoint-operator based approaches to sensitivity analysis were functionals. However, in many problems of practical interest, the response can no longer be represented by a functional, but needs to be represented by a more general operator. Time- and/or space-dependent responses, for example, need to be represented by operators. A general representation of an operator-type response is considered in Sec. III. In this section, a general formulation of sensitivity theory that is capable of treating such operator-type responses is developed by using several of the concepts and results established in Ref. 1. Finally, Sec. IV summarizes the theoretical advances which this work contributes to sensitivity theory.

Although this work extends the theory formulated in Ref. 1 by considering more general classes of responses, the physical problem is the same as in Ref. 1. It is helpful to recall that this problem is represented, for the sake of generality, by the following system of K coupled nonlinear equations written in operator form as

$$\mathbf{N}[u(x),\alpha(x)] = \mathbf{Q}[\alpha(x),x]. \tag{1}$$

The quantities appearing in Eq. (1) are defined as follows:

1. $x = (x_1,\cdots,x_J)$ is the phase-space position vector;

[a)]Research sponsored by Electric Power Research Institute (RP 1441-1) subcontract with Oak Ridge National Laboratory, operated by Union Carbide Corporation for the U.S. Department of Energy.

 0022-2488/81/122803-10$01.00

$x \in \Omega \subset \mathscr{R}^J$, where Ω is subset of the J-dimensional real vector space $\mathscr{R}^J$,

2. $u(x) = [u_1(x),\cdots,u_K(x)]$ is the state vector; $u(x) \in E_u$, where E_u is a normed linear space over the scalar field Λ of real numbers,

3. $\alpha(x) = [\alpha_1(x),\cdots,\alpha_I(x)]$ is the vector of system parameters; $\alpha \in E_\alpha$, where E_α is also a normed linear space,

4. $\mathbf{Q}[\alpha(x),x] = [Q_1(\alpha,x),\cdots,Q_K(\alpha,x)]^T$ is a (column) vector whose elements represent inhomogeneous source terms (the symbol T denoted "transposition"); $\mathbf{Q} \in E_Q$, where E_Q is again a normed liner space. The components of $\mathbf{Q}$ may be operators (rather than just functions) acting on $\alpha(x)$ and x,

5. the components of the (column) vector $\mathbf{N} = [N_1(u,\alpha),\cdots,N_K(u,\alpha)]^T$ are nonlinear operators acting, in general, not only on the state vector $u(x)$, but also on the vector of system parameters $\alpha(x)$.

In view of these definition, $\mathbf{N}$ represents the mapping $\mathbf{N}: S \subset E \to E_Q$, where $S = S_u \times S_\alpha, S_u \subset E_u, S_\alpha \subset E_\alpha$, and $E = E_u \times E_\alpha$. Note that an arbitrary element $e \in E$ is of the form $e = (u,\alpha)$. If differential operators appear in Eq. (1), then a corresponding set of boundary conditions —which is essential to define the domain S of $\mathbf{N}$—must also be given. This set can be represented as

$$\{\mathbf{B}(e) - \mathbf{A}(\alpha)\}_{\partial\Omega} = \mathbf{O}, \tag{2}$$

where $\mathbf{A}$ and $\mathbf{B}$ are operators and $\partial\Omega$ is the boundary of Ω; the operator $\mathbf{A}(\alpha)$ represents all inhomogeneous boundary terms.

The specifications introduced so far are sufficiently general to allow Eqs. (1) and (2) to include, as particular cases, the mathematical modeling of a wide range of problems of practical interest in many diverse fields. Still remaining to be defined is the system response associated with the problem modeled by Eqs. (1) and (2).

II. SYSTEM RESPONSE: A FUNCTIONAL DEFINED AT A CRITICAL POINT OF A FUNCTION OF THE SYSTEM'S STATE VECTOR AND PARAMETERS

Consider the system response R to be a functional of $e = (u,\alpha)$ defined at a critical point $y(\alpha)$ of a function $F(u,x,\alpha)$. Such a response can be represented as a functional of the form

$$R(e) = \int_\Omega F(u,x,\alpha) \prod_{i=1}^{M} \delta[x_i - y_i(\alpha)] \prod_{j=M+1}^{J} \delta(x_j - z_j)\, dx. \tag{3}$$

The quantities appearing in the integrand of Eq. (3) are defined as follows:

1. F is the nonlinear function under consideration,

2. $\delta(x)$ is the customary "delta" functional,

3. $\alpha \in \mathscr{R}^I$, i.e., the components α_i, $i = 1,\cdots,I$, are restricted throughout this section to be real numbers;

4. $y(\alpha) = [y_1(\alpha),\cdots, y_M(\alpha)]$, $M \leqslant J$, is a critical point of F. This critical point is defined here in one of the following two ways:

(a) If the G differential of F vanishes at $y(\alpha)$, then $y(\alpha)$ is a critical point defined implicitly as the solution of the system of equations

$$\{\partial F/\partial x_i\}_{y(\alpha)} = 0; \quad i = 1,\cdots, J. \tag{4}$$

In this case, $y(\alpha)$ has J components (i.e., $M = J$), and $\Pi_{j=M+1}^{J} \delta(x_j - z_j) \equiv 1$ in the integrand of Eq. (3). Note that, in general, $y(\alpha)$ is a function of α.

(b) Occasionally, it may happen that $\partial F/\partial x_j$ takes on nonzero constant values (i.e., values that do not depend on x) for some of the variables x_j, $j = M+1,\cdots, J$. Then, as a function of these variable x_j, F attains its extreme values at the points $x_j = z_j$, $z_j \in \partial\Omega$. Evaluating F at z_j, $j = M+1,\cdots,J$, yields a function G which depends on the remaining phase-space variables x_i, $i = 1,\cdots, M$; G may then have a critical point at $y(\alpha) = [y_1(\alpha),\cdots,y_M(\alpha)]$ defined implicitly as the solution of

$$\{\partial G/\partial x_i\}_{y(\alpha)} = 0; \quad i = 1,\cdots, M. \tag{5}$$

With the above specifications, the definition of $R(e)$ given in Eq. (3) is sufficiently general to include treatment of extrema (local, relative, or absolute), saddle, and inflexion points of the function F of interest. In practice, the base-case solution path, and therefore the specific nature and location of the critical point under consideration, are completely known prior to initiating the sensitivity studies.

It is thus apparent that in the formulation of a complete sensitivity theory, the components $y_i(\alpha)$, $i = 1,\cdots,M$, must be treated as responses in addition to $R(e)$. Hence, the objective of this sensitivity theory is twofold:

1. to determine the G differential $VR(e^0;h)$ of $R(e)$ at the "base-case configuration point" $e^0 = (u^0, \alpha^0)$, which gives the sensitivity of $R(e)$ to changes $h = (h_u, h_\alpha)$ in the systems state functions and parameters, and

2. to determine the (column) vector $Vy(\alpha^0;h_\alpha) = (Vy_1,\cdots, Vy_M)$ whose components $Vy_m(\alpha^0;h_\alpha)$ are the G differentials of $y_m(\alpha)$ at α^0, for $m = 1,\cdots,M$. The vector $Vy(\alpha^0;h_\alpha)$ gives the sensitivity of the critical point $y(\alpha)$ to changes h_α.

To achieve the objective mentioned above, the two alternative formalisms, the "forward sensitivity formalism" and the "adjoint sensitivity formalism", are developed along the same general lines as discussed in detail in Ref. 1.

A. The "forward sensitivity formalism"

Applying the definition of the G differential to Eq. (3) shows that

$$VR(e^0;h) = \int_\Omega [F'_u(e^0)h_u + F'_\alpha(e^0)h_\alpha] \prod_{i=1}^{M} \delta[x_i - y_i(\alpha^0)] \prod_{j=M+1}^{J} \delta(x_j - z_j)\, dx$$
$$+ \sum_{m=1}^{M} \left[-h_\alpha \left(\frac{dy_m}{d\alpha} \right)_{\alpha^0} \right] \int_\Omega F\delta'(x_m - y_m) \prod_{i=1, i\neq m}^{M} \delta(x_i - y_i) \prod_{j=M+1}^{J} \delta(x_j - z_j)\, dx. \tag{6}$$

The last term on the right side of Eq. (6) vanishes, since

$$\int_\Omega F\delta'(x_m - y_m) \prod_{i=1,i\neq m}^{M} \delta(x_i - y_i) \prod_{j=M+1}^{J} \delta(x_j - z_j)\, dx = -\int_\Omega (\partial F/\partial x_m) \prod_{i=1}^{M} \delta(x_i - y_i) \prod_{j=M+1}^{J} \delta(x_j - z_j)\, dx = 0,$$

$m = 1,\cdots,M,$ (7)

in view of the well-known definition of the δ' functional and in view of either Eq. (4) if $M = J$, or of Eq. (5) if $M < J$. Therefore, the expression of $VR(e^0;h)$ simplifies to

$$VR(e^0;h) = \int_\Omega [F'_u(e^0)h_u + F'_\alpha(e^0)h_\alpha] \prod_{i=1}^{M} \delta[x_i - y_i(\alpha^0)] \prod_{j=M+1}^{J} \delta(x_j - z_j)\, dx. \tag{8}$$

Thus, the sensitivity $VR(e^0;h)$ of $R(e)$ to specified changes h_α can in principle be evaluated once the vector h_u is determined from the "forward sensitivity equations"[1], i.e.,

$$\left.\begin{aligned} &V\mathbf{N}(u^0,\alpha^0;h_u,h_\alpha) - V\mathbf{Q}(\alpha^0;h_\alpha) = \mathbf{0}, \\ &\{V\mathbf{B}(u^0,\alpha^0;h_u,h_\alpha) - V\mathbf{A}(\alpha^0;h_\alpha)\}_{\partial\Omega} = \mathbf{0} \end{aligned}\right\} \tag{9}$$

As already mentioned, the sensitivity of the location in phase space of the critical point is given by the G differential $Vy(\alpha^0;h_\alpha)$ of $y(\alpha)$ at α^0. In view of either Eq. (4) or Eq. (5), each of the components $y_1(\alpha),\cdots,y_M(\alpha)$ of $y(\alpha)$ is a real-valued function of the real variables $\alpha_1,\cdots,\alpha_I$, and may be viewed as a functional defined on a subset of $\mathscr{R}^I$. Therefore, each G differential $Vy_m(\alpha^0;h_\alpha)$ of $y_m(\alpha)$ at α^0 is given by

$$Vy_m(\alpha^0;h_\alpha) = \left\{\frac{dy_m}{d\alpha}\right\}_{\alpha^0} \cdot h_\alpha = \sum_{i=1}^{I} \left\{\frac{\partial y_m}{\partial \alpha_i}\right\}_{\alpha^0} h_{\alpha_i}; \quad m = 1,\cdots,M, \tag{10}$$

provided that $\partial y_m/\partial\alpha_i, i = 1,\cdots,I$, exist at α^0 for all $m = 1,\cdots,M$.

The explicit expression of $Vy(\alpha^0;h_\alpha)$ is obtained as follows. First, it is observed that both Eq. (4) and Eq. (5) can be represented as

$$\int_\Omega (\partial F/\partial x_m) \prod_{i=1}^{M} \delta[x_i - y_i(\alpha)] \prod_{j=M+1}^{J} \delta(x_j - z_j)\, dx = 0; \quad m = 1,\cdots,M. \tag{11}$$

Taking the G differential of Eq. (11) at e^0 yields the following system of equations involving the components Vy_m:

$$\int_\Omega \{\partial(F'_u h_u + F'_\alpha h_\alpha)/\partial x_m\}_{e^0} \prod_{i=1}^{M} \delta[x_i - y_i(\alpha^0)] \prod_{j=M+1}^{J} \delta(x_j - z_j)\, dx$$

$$- \sum_{s=1}^{M} Vy_s(\alpha^0;h_\alpha) \int_\Omega \{\partial F/\partial x_m\}_{e^0} \delta'[x_s - y_s(\alpha^0)] \prod_{i=1,i\neq s}^{M} \delta[x_i - y_i(\alpha^0)] \prod_{j=M+1}^{J} \delta(x_j - z_j)\, dx = 0; \quad m = 1,\cdots,M. \tag{12}$$

The above system is algebraic and linear in the components $Vy_s(\alpha^0;h_\alpha)$; therefore, it can be represented in matrix form as

$$\Phi Vy = \Gamma \tag{13}$$

by defining $\Phi = [\phi_{ms}]$ to be the $M \times M$ matrix with elements

$$\phi_{ms} \equiv \int_\Omega \{\partial^2 F/\partial x_m \partial x_s\}_{e^0} \prod_{i=1}^{M} \delta[x_i - y_i(\alpha^0)] \prod_{j=M+1}^{J} \delta(x_j - z_j)\, dx, \quad \text{for } m,s = 1,\cdots,M. \tag{14}$$

and by defining Γ to be the M-component (column) vector

$$\Gamma(f_1 + g_1,\cdots,f_M + g_M)^T, \tag{15}$$

where

$$f_m \equiv -\int_\Omega \{\partial(F'_\alpha h_\alpha)/\partial x_m\}_{e^0} \prod_{i=1}^{M} \delta[x_i - y_i(\alpha^0)] \prod_{j=M+1}^{J} \delta(x_j - z_j)\, dx; \quad m = 1,\cdots,M, \tag{16}$$

and

$$g_m \equiv -\int_\Omega \{\partial(F'_u h_u)/\partial x_m\}_{e^0} \prod_{i=1}^{M} \delta[x_i - y_i(\alpha^0)] \prod_{j=M+1}^{J} \delta(x_j - z_j)\, dx; \quad m = 1,\cdots,M. \tag{17}$$

Notice that the definition of the δ' functional has been used to recast the second integral in Eq. (12) into the equivalent expression given in Eq. (14).

As this stage, the quantities ϕ_{ms} and f_m can be evaluated most efficiently by directly using Eqs. (14) and (16). It is of interest to observe here that if $M = J$, then Φ is the Hessian of F evaluated at the critical point $y(\alpha^0)$; alternatively, if $M < J$, then Φ is the Hessian of the function G [considered in Eq. (5)] evaluated at the respective critical point. The quantities g_m defined in Eq. (17) can also be evaluated, since h_u will have already been determined to compute the sensitivity $VR(e^0;h)$ given in Eq. (8). Upon completing the computation of the elements of Φ and Γ, Eq. (13) can be solved by employing methods of linear algebra to obtain

$$Vy(\alpha^0;h_\alpha) = \Phi^{-1}\Gamma. \tag{18}$$

As underscored by the derivations presented so far, the availability of the solution h_u of the "forward sensitivity equations" given in Eq. (9) is essential to evaluate both $VR\,(e^0;h\,)$ and $Vy(\alpha^0;h_\alpha)$. This is a distinctive characteristic of the "forward sensitivity formalism" which, from an economical standpoint, makes this formalism ill-suited for sensitivity analysis of problems with large data bases (i.e., when α has many components).

B. The "adjoint sensitivity formalism"

Since most of the problems encountered in practice are characterized by large data bases, the development of this formalism is motivated by the need for a tool to perform sensitivity analyses of such problems economically. To this end, the development of this formalism is centered on eliminating the explicit appearance of the unknown values of the vector h_u from Eqs. (8) and (18), and hence on circumventing the need to repeatedly solve Eq. (9). However, as detailed in Ref. 1, h_u can be eliminated if and only if (iff) the following conditions are satisfied:

(C.1) the partial G derivatives at e^0 of $R\,(e)$ with respect to u and α exist,

(C.2) the partial G derivatives at e^0 of the operators $\mathbf{N}$ and $\mathbf{B}$ with respect to u and α exist,

(C.3) the spaces E_u and E_Q are real Hilbert spaces, denoted by H_u and H_Q, respectively. For $u_1,u_2\in H_u$, the inner product in H_u will be denoted by $[u_1,u_2]$, and is given by the integral $\int_\Omega u_1\cdot u_2\,dx$. The inner product in H_Q will be denoted by $\langle\ ,\ \rangle$.

An examination of Eq. (8) shows that $VR\,(e^0;h\,)$ is linear in h. Hence, condition (C.1) is satisfied, and the H_u-dependent component of $VR\,(e^0;h\,)$, i.e., the "indirect effect term," can be written in inner product form as

$$\int_\Omega F'_u(e^0)h_u \prod_{i=1}^{M}\delta[x_i - y_i(\alpha^0)] \prod_{j=M+1}^{J}\delta(x_j - z_j)\,dx = [\nabla_u R\,(e^0),h_u\,], \tag{19}$$

where

$$\nabla_u R\,(e^0) = \prod_{i=1}^{M}\delta[x_i - y_i(\alpha^0)] \prod_{j=M+1}^{J}\delta(x_j - z_j) \times\left(\frac{\partial F(e^0)}{\partial u_1},\cdots,\frac{\partial F(e^0)}{\partial u_K}\right)^T. \tag{20}$$

The adjoint system is constructed by following the procedure set forth in Ref. 1. (For brevity, details are omitted here.) Thus, condition (C.2) makes it possible to write the system of equations given in Eq. (9) as

$$\mathbf{N}'_u(e^0)h_u = V\mathbf{Q}(\alpha^0;h_\alpha) - \mathbf{N}'_\alpha(e^0)h_\alpha \tag{21}$$

and

$$\{\mathbf{B}'_u(e^0)h_u\}_{\partial\Omega} = \{V\mathbf{A}(\alpha^0;\mathrm{h}_\alpha) - \mathbf{B}'_\alpha(e^0)h_\alpha\}_{\partial\Omega}. \tag{22}$$

Next, in view of Eq. (21) and condition (C.3), the following relationship holds for a vector $v\in H_Q$:

$$\langle v,\mathbf{N}'_u(e^0)h_u\rangle = [\mathbf{L}^*(e^0)v,h_u\,] + \{P\,[h_u;v]\}_{\partial\Omega}, \tag{23}$$

where $\mathbf{L}^*(e^0)$ is the operator formally adjoint to $\mathbf{N}'_u(e^0)$, and $\{P\,[h_u;v]\}_{\partial\Omega}$ is the associated bilinear form evaluated on $\partial\Omega$. The domain of $\mathbf{L}^*(e^0)$ is determined by selecting appropriate adjoint boundary conditions, represented here in operator form as

$$\{\mathbf{B}^*(v;e^0) - \mathbf{A}^*(e^0)\}_{\partial\Omega} = \mathbf{0}. \tag{24}$$

These boundary conditions are obtained by requiring that

1. they be independent of h_u,h_α, and G derivatives with respect to α, and

2. the substitution of Eqs. (22) and (24) into the expression of $\{P\,[h_u;v]\}_{\partial\Omega}$ must cause all terms containing unknown values of h_u to vanish.

This selection of the adjoint boundary conditions reduces $\{P\,[h_u;v]\}_{\partial\Omega}$ to a quantity designated here by $\hat{P}(h_\alpha,v;e^0)$, where $\hat{P}$ contains boundary terms involving only known values of h_α,v, and (possibly) e^0. In general, $\hat{P}$ does not automatically vanish as a result of these manipulations,[1] although it may do so in particular instances. Hence, Eq. (23) can be written as

$$[\mathbf{L}^*(e^0)v,\,h_u\,] = \langle v,V\mathbf{Q}(\alpha^0;h_\alpha) - \mathbf{N}'_\alpha(e^0)h_\alpha\rangle - \hat{P}(h_\alpha,v;e^0), \tag{25}$$

where Eq. (21) was used to replace $\mathbf{N}'_u(e^0)h_u$. Comparing the left-hand side of Eq. (25) with the right-hand side of Eq. (19) shows that

$$\mathbf{L}^*(e^0)v = \nabla_u R\,(e^0). \tag{26}$$

Note that the uniqueness of the above relationship is ensured by the Riesz representation theorem.[2] This completes the construction of the adjoint system. Furthermore, Eqs. (19), (25), and (26) can be used to express Eq. (8) as

$$VR\,(e^0;h\,) = \int_\Omega F'_\alpha(e^0)h_\alpha \prod_{i=1}^{M}\delta[x_i - y_i(\alpha^0)] \prod_{j=M+1}^{J}\delta(x_j - z_j)\,dx + \langle V\mathbf{Q}(\alpha^0;h_\alpha) - \mathbf{N}'_\alpha(e^0)h_\alpha,v\rangle - \hat{P}(h_\alpha,v;e^0). \tag{27}$$

The desired elimination of the unknown values of h_u from the expression giving the sensitivity $VR\,(e^0;h\,)$ has thus been accomplished.

Unknown values of h_u can be eliminated from the expression of $Vy(\alpha^0;h_\alpha)$ given in Eq. (18), only if they can be eliminated from appearing in Eq. (17). Examination of Eq. (17) reveals that each quantity g_m is a functional that can be expressed in the equivalent form

$$g_m = \int_\Omega F'_u(e^0)h_u\delta'(x_m - y_m) \times \prod_{i=1,i\neq m}^{M}\delta(x_i - y_i) \prod_{j=M+1}^{J}\delta(x_j - z_j)\,dx. \tag{28}$$

by employing the definition of the δ' functional. In turn, the above expression can be written as the inner product

$$g_m = [\gamma_m(e^0),h_u\,], \tag{29}$$

where

$$\gamma_m(e^0) \equiv \delta'[\dot{x}_m - y_m(\alpha^0)] \prod_{i=1,i\neq m}^{M}\delta(x_i - y_i) \times \prod_{j=M+1}^{J}\delta(x_j - z_j)\left(\frac{\partial F(e^0)}{\partial u_1},\cdots,\frac{\partial F(e^0)}{\partial u_k}\right)^T. \tag{30}$$

The desired elimination of the unknown values of h_u from Eq. (29) can now be accomplished by letting each of the functions $\gamma_m(e^0)$ play, in turn, the role previously played by $\nabla_u R(e^0)$ [cf. Eq. (20)], and by following the same procedure as that leading to Eq. (27). The end result is

$$g_m = \langle V\mathbf{Q}(\alpha^0;h_\alpha) - \mathbf{N}'_\alpha(e^0)h_\alpha, w_m\rangle - \hat{P}(h_\alpha,w_m;e^0), \tag{31}$$

where each function w_m is the solution of the adjoint system

$$\left.\begin{aligned} &\mathbf{L}^*(e^0)w_m = \gamma_m(e^0) \\ &\{\mathbf{B}^*(w_m;e^0) - \mathbf{A}^*(e^0)\}_{\partial\Omega} = \mathbf{0} \end{aligned}\right\} \tag{32}$$

for $m = 1,\cdots,M$.

It is important to note that $\mathbf{L}^*(e^0)$,$\mathbf{B}^*(e^0)$, and $\mathbf{A}^*(e^0)$ appearing in Eq. (32) are the same operators as those appearing in Eqs. (26) and (24). Only the source term $\gamma_m(e^0)$ in Eq. (32) differs from the corresponding source term $\nabla_u R(e^0)$ in Eq. (26). Therefore, the computer code employed to solve the adjoint system given in Eqs. (26) and (24) can be used, with relatively trivial modifications, to compute the functions w_m from Eq. (32). Comparing now the right sides of Eqs. (25) and (31) reveals that the quantity $\hat{P}(h_\alpha,v;e^0)$ is formally identical to the quantity $\hat{P}(h_\alpha,w_m;e^0)$, and that the function $V\mathbf{Q}(\alpha^0;h_\alpha) - \mathbf{N}'_\alpha(e^0)h_\alpha$ appears in both the inner products denoted by $\langle\ ,\ \rangle$. This indicates that the computer program employed to evaluate the second and third terms on the right side of Eq. (27) can also be used to evaluate the functionals g_m, $m = 1,\cdots, M$, given in Eq. (31). Of course, the values of v required to compute $VR(e^0;h)$ are to be replaced by the respective values of w_m when computing the g_m's.

In most practical problems, the total number of parameters I greatly exceeds the number of phase-space variables J, and hence M, since $M \leqslant J$. Therefore, if the "adjoint sensitivity formalism" can be developed as described in this section, then a large amount of computing costs can be saved by employing this formalism rather than the "forward sensitivity formalism." In the case, only $M + 2$ "large" computations (one for the "base-case," one for the adjoint function v, and M for the adjoint functions $w_1,\cdots,w_M$) are needed to obtain the sensitivities $VR(e^0;h)$ and $Vy(\alpha^0;h_\alpha)$ to changes in *all* of the parameters. By contrast $I + 1$ computations (one for the "base-case," and I to obtain the vector h_u) would be required if the "forward sensitivity formalism" were employed.

C. Discussion

Note that, as shown in Eqs. (6)–(8), the contributions to $VR(e^0;h)$ arising from the α dependence of $y(\alpha)$ vanish only because $y(\alpha)$ is a critical point of F. An important consequence of this fact can be demonstrated by *considering the point y not to be a function of* α. The response would then take on the form

$$R_1(e) = \int_\Omega F(u,x,\alpha)\prod_{i=1}^{M}\delta(x_i - y_i)\prod_{j=M+1}^{J}\delta(x_j - z_j)\,dx. \tag{33}$$

In the above equation, the subscript 1 indicates that the mathematical characteristics of $R_1(e)$ differ from those of $R(e)$, although both responses take on identical values at $e = e^0$, i.e.,

$$R_1(e^0) = R(e^0). \tag{34}$$

Calculating the G differential $VR_1(e^0;h)$ of $R_1(e)$ at e^0 gives

$$VR_1(e^0;h) = \int_\Omega [F'_u(e)h_u + F'_\alpha(e^0)h_\alpha]\prod_{i=1}^{M}\delta(x_i - y_i) \times \prod_{j=M+1}^{J}\delta(x_j - z_j)\,dx. \tag{35}$$

Comparison of Eqs. (35) and (8) shows that

$$VR_1(e^0;h) = VR(e^0;h). \tag{36}$$

Consider now the total variations of $R(e)$ and $R_1(e)$ at $e = e^0$, i.e.,

$$R(e^0 + h) - R(e^0) = VR(e^0;h) + \Delta(h), \quad \text{where}$$
$$\lim_{t\to 0}[\Delta(th)/t] = 0, \tag{37}$$

and

$$R_1(e^0 + h) - R_1(e^0) = VR_1(e^0;h) + \Delta_1(h), \quad \text{where}$$
$$\lim_{t\to 0}[\Delta_1(th)/t] = 0. \tag{38}$$

Substracting Eq. (38) from Eq. (37) and taking into account Eqs. (34) and (36), yields the relationship

$$R(e^0 + h) - R_1(e^0 + h) = \varepsilon(h), \quad \text{where}$$
$$\lim_{t\to 0}[\varepsilon(th)/t] = 0. \tag{39}$$

The result given in Eq. (39) can be readily be strengthened if R is Fréchet differentiable [i.e., if $VR(e^0;h)$ is continuous and linear in h at e^0, and is continuous in e at e^0]. In such a case, R_1 is also Fréchet differentiable; hence, $\lim_{t\to 0}[\Delta(th)/t] = 0$ in Eq. (37) and $\lim_{t\to 0}[\Delta_1(th)/t] = 0$ in Eq. (38) hold uniformly with respect to h on the set $\{h:||h|| = 1\}$. Consequently, $\lim_{t\to 0}[\varepsilon(th)/t] = 0$ in Eq. (39) also holds uniformly with respect to h on $\{h:||h|| = 1\}$, and can be written in the equivalent form $\lim_{h\to 0}[||\varepsilon(h)||/||h||] = 0$. Thus, the stronger result

$$||R(e^0 + h) - R_1(e^0 + h)|| = O(||h||^2) \tag{40}$$

holds if R is Fréchet differentiable at $e = e^0$.

A simple illustration of the distinctions between $R(e)$ and $R_1(e)$ is shown in Fig. 1. There, the critical point $y_1(\alpha)$ of $F(u,x,\alpha)$ is a maximum occurring in the (one-dimensional) direction x_1. Changes $h = (h_u,h_\alpha)$ would cause the new maximum of F to take on the value $R(e^0 + h)$ at $y_1(\alpha^0 + h_\alpha)$. The sensitivity $VR(e^0;h)$ of $R(e)$ at e^0 is given by Eq. (8) [or Eq. (27)], while the sensitivity $Vy_1(\alpha^0;h_\alpha)$ of $y_1(\alpha)$ at α^0 is given by Eq. (18). However, if y_1 is considered *not* to be a function of α, then $R_1(e^0 + h)$ would be the altered value of the functional $R_1(e)$. Nevertheless, the sensitivity $VR_1(e^0;h)$ of $R_1(e)$ at e^0 is the same as the sensitivity $VR(e^0;h)$ of $R(e)$ at e^0, as shown in Eq. (36). This is only because $y_1(\alpha)$ is a critical point of $F(u,x,\alpha)$.

The foregoing discussion sheds additional light on the proper interpretation of the results presented in Refs. 3,4,5, and 6. On the one hand, responses designated as "peak fuel

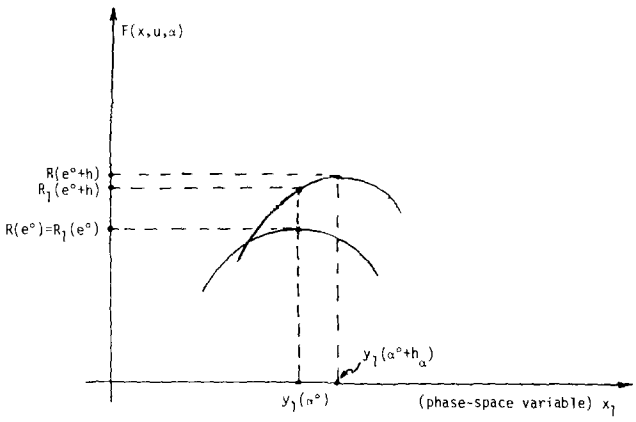

FIG. 1. Illustration of the distinction between $R(e)$ and $R_1(e)$.

temperature," "peak clad temperature," etc., were considered for sensitivity studies in Refs. 3 and 4. In that context, the qualifier "peak" signified only that those responses were located at the position in phase-space where the maximum of the respective state function (in particular, the temperature) occured in the "base-case" calculation; the position itself was considered to remain unchanged regardless of variations h_{α_i} in the system parameters α_i. It is therefore apparent that the aforementioned responses are, in fact, particular forms of $R_1(e)$ [cf. Eq. (33)]. On the other hand, the "maximum cladding temperature" response considered in Refs. 5 and 6 is a particular form of $R(e)$ [cf. Eq. (3)].

Further insight regarding the distinctions between $R(e)$ and $R_1(e)$ is provided by a brief comparative analysis of selected sensitivity analysis results reported in Refs. 4 and 5 for a thermal-hydraulics sample problem. It is recalled that this sample problem models a Clinch River Breeder Reactor fuel rod, subjected to a power transient, in a sodium-filled coolant channel. To facilitate this comparative analysis, sensitivity results for the "maximum cladding temperature" response considered in Ref. 5 and for the "peak cladding temperature" response considered in Ref. 4 are reproduced below in Tables I and II, respectively. (For brevity, only results corresponding to the most significant system parameters are reproduced here.)

Note that for both of these responses, the function F [cf. Eqs. (3) and (33)] is the space- and time-dependent temperture [i.e., $F(u,x,\alpha) = u \equiv T(r,z,t)$]. Identical numerical methods were employed in both Refs. 4 and 5 to solve the system of nonlinear partial differential equations modeling this problem, to solve the adjoint system, and to evaluate the sensitivities $VR(e^0;h)$ and $VR_1(e^0;h)$. Note also that in Tables I and II, for every value of the index i,h is still given by $h = (h_u, h_\alpha)$, but all the components of h_α are zero except for h_{α_i}.

As expected from Eq. (36) and as confirmed by comparing the results given in Tables I and II under the heading "relative sensitivity," the sensitivities corresponding to a particular system parameter α_i are identical. Also, the expected identity between the corresponding results given in these tables under the heading "predicted perturbed response" is confirmed. However, the results shown in Table I under the heading "recalculated perturbed response" are not identical to the corresponding results shown in Table II.

TABLE I. Sensitivity results for maximum cladding temperature response. Unperturbed response $R(e^0) = 568$°C.

i	Parameter (α_i)	Relative sensitivity [a]	$\frac{h_{\alpha_i}}{\alpha_i}$	Predicted perturbed response [b] (°C)	Recalculated perturbed response [c] (°C)
1	fuel outer radius	4.4670	0.01	594	600
			−0.01	543	546
2	gap outer radius	−4.4123	0.01	543	547
			−0.01	593	599
3	inlet coolant temperature	0.5239	0.10	598	598
			0.25	643	643
4	coolant mass flow rate	−0.2602	−0.10	583	584
			0.10	553	555
5	gap width (at constant clad thickness)	−0.1426	0.25	548	550
			−0.25	588	593
6	gap conductance	0.1421	0.10	576	576
			−0.10	560	560
7	fuel heat source	0.0632	0.10	572	572
			−0.10	565	565
8	clad outer radius	0.0568	0.05	570	569
			−0.05	567	567
9	axial discretization parameter	−0.2170	0.10	556	557

[a] Relative sensitivity $[VR(e^0;h)/R(e^0)][\alpha_i^0/h_{\alpha_i}]$.

[b] Predicted perturbed response $\equiv R(e^0) + VR(e^0;h)$.

[c] Recalculated perturbed response $\cong R(e^0 + h)$.

TABLE II. Sensitivity results for peak cladding temperature response. Unperturbed response $R_1(e^0) = 568$ °C.

i	Parameter (α_i)	Relative sensitivity [a]	$\frac{h_{\alpha_i}}{\alpha_i}$	Predicted perturbed response [b] (°C)	Recalculated perturbed response [c] (°C)
1	fuel outer radius	4.4670	0.01	594	597
			−0.01	543	546
2	gap outer radius	−4.4123	0.01	543	546
			−0.01	593	597
3	inlet coolant temperature	0.5239	0.10	598	598
			0.25	643	643
4	coolant mass flow rate	−0.2602	−0.10	583	584
			0.10	553	555
5	gap width (at constant clad thickness)	−0.1426	0.25	548	550
			−0.25	588	591
6	gap conductance	0.1421	0.10	576	576
			−0.10	560	560
7	fuel heat source	0.0632	0.10	572	572
			−0.10	565	565
8	clad outer radius	0.0568	0.05	570	570
			−0.05	567	567
9	axial discretization parameter	−0.2170	0.10	556	557

[a] Relative sensitivity $\equiv [\mathcal{V}R_1(e^0;h)/R_1(e^0)]\,[\alpha_i^0/h_{\alpha_i}]$.

[b] Predicted perturbed response $\equiv R_1(e^0) + \mathcal{V}R_1(e^0;h)$.

[c] Recalculated perturbed response $\equiv R_1\{e^0 + h\}$.

According to Eq. (40), the differences between the two recalculated results for a particular parameter α_i arise from the second- and higher-order effects caused by variations h_{α_i} around the "base-case" value α_i^0. These second- and higher-order effects are very small for this particular sample problem. Note that the theory developed in Secs. IIA and IIB was also successfully applied in Refs. 5 and 6 to determine the sensitivities of the location in phase-space of the "maximum cladding temperature."

III. SYSTEM RESPONSES: OPERATORS

To date, the system responses considered in adjoint-function based approaches to sensitivity analysis were functionals, i.e., particular types of operators mapping domains in $E = E_u \times E_\alpha$ into the underlying field of real scalars Λ. However, in many practical problems, the system response is a more general operator whose range is not in Λ but in some other normed linear space E_R. Examples of such responses are time and/or space dependent mappings involving the system's state vector and parameters. Using the same notation as introduced in Sec. I, a member of this class of responses can generally by represented as

$$\mathbf{R}(e): D \subset E \to E_R. \tag{41}$$

A. Sensitivity theory

As before,[1] the sensitivity of $\mathbf{R}(e)$ to "changes" h_α in the system parameters α is defined as the Gâteaux differential $\mathcal{V}\mathbf{R}(e^0;h)$ of $\mathbf{R}(e)$ at e^0 with increment $h = (h_u, h_\alpha)$. It is recalled that the definition of $\mathcal{V}\mathbf{R}(e^0;h)$ is

$$\mathcal{V}\mathbf{R}(e^0;h) = \lim_{t \to 0} [\mathbf{R}(e^0 + th) - \mathbf{R}(e^0)]/t \tag{42}$$

for $t \in \Lambda$ and $h \in E$.

In view of Eqs. (42) and (9), it becomes apparent that although the response is now an operator rather than just a functional, the necessary and sufficient conditions underlying the "forward sensitivity formalism" are not affected. (Recall[1] that these conditions require the existence of the G differentials at e^0 of the operators appearing in the definition of the problem, including the response.) Thus, for a specified vector of "changes" h_α, $\mathcal{V}\mathbf{R}(e^0;h)$ can in principle be evaluated once the vector h_u is determined from Eq. (9).

As previously discussed, most of the computational expense of using the forward sensitivity formalism arises from repeatedly solving Eq. (9) to determine h_u for all possible vectors h_α. Hence, for a given problem, the cost of computing sensitivities for an operator response is essentially the same as that for a functional response, if the forward sensitivity formalism is used in both cases.

As discussed in Ref. 1, the practical motivation underlying the development of the alternative "adjoint sensitivity formalism" is to avoid the need to repeatedly solve Eq. (9). This required the elimination of all unknown values of h_u from the expression of $\mathcal{V}\mathbf{R}(e^0;h)$. In turn, this elimination intrinsically relied on $\mathcal{V}\mathbf{R}(e^0;h)$ being a functional, enabling the construction of the appropriate adjoint system using inner products. However, the adjoint sensitivity formalism developed in Ref. 1 is restricted to responses that are functionals; for this reason, it will henceforth be referred to as the "adjoint sensitivity formalism for functionals."

Although $\mathcal{V}\mathbf{R}(e^0;h)$ defined in Eq. (42) is an operator rather than just a functional, the analysis[1] of the necessary

and sufficient conditions underlying the validity of the adjoint sensitivity formalism for functionals establishes guidelines for a similar formalism for operator responses (henceforth called the "adjoint sensitivity formalism for operators").

In this way, the following guidelines for developing the adjoint sensitivity formalism for operators emerge:

(G.1) isolate the h_u dependence of $V\mathbf{R}(e^0;h)$ from the functional dependence of $V\mathbf{R}(e^0;h)$ on the remaining quantities,

(G.2) express the quantity containing this h_u dependence in the form of linear combinations of functionals that are themselves linear in h_u,

(G.3) employ the adjoint sensitivity formalism for functionals to evaluate the functionals determined in item (G.2) above.

The development of these guidelines into a rigorous formalism will necessarily involve the use of adjoint operators. Since adjoint operators in Hilbert spaces are more convenient to deal with than adjoint operators in Banach spaces, subsequent development are facilitated by taking advantage of the simplifying geometrical properties of Hilbert spaces while still retaining sufficient generality for practical applications. In this vein, the spaces E_u, E_Q, and E_R are henceforth considered Hilbert spaces and denoted as $H_u(\Omega)$, $H_Q(\Omega)$ and $H_R(\Omega_R)$, respectively. The elements of $H_u(\Omega)$ and $H_Q(\Omega)$ are, as before, vector functions defined on the open set $\Omega \subset \mathscr{R}^J$ with the smooth boundary $\partial\Omega$. The elements of $H_R(\Omega_R)$ are vector or scalar functions defined on the open set $\Omega_R \subset \mathscr{R}^m, 1 \leqslant m \leqslant J$, with a smooth boundary $\partial\Omega_R$. (Of course, if $J = 1$, then $\partial\Omega$ merely consists of two endpoints; similarly, if $m = 1$, then $\partial\Omega_R$ consists of two endpoints only.) The inner products on $H_u(\Omega)$, $H_Q(\Omega)$, and $H_R(\Omega_R)$ are denoted by $[\,,\,]$, $\langle\,,\,\rangle$, and $\{\,,\,\}$, respectively.

In view of the foregoing guidelines (G.1) and (G.2), it becomes apparent that further progress is possible only if $V\mathbf{R}(e^0;h)$ is linear in h. Applying a theorem proved by Vainberg[7] readily shows that $V\mathbf{R}(e^0;h)$ is linear in h if and only if (iff)

$$\left.\begin{aligned}&\text{(a) } \mathbf{R}(e) \text{ satisfies a weak Lipschitz condition at } e^0, \text{ and}\\ &\text{(b) } \mathbf{R}(e^0 + th_1 + th_2) - \mathbf{R}(e^0 + th_1) - \mathbf{R}(e^0 + th_2)\\ &\qquad + \mathbf{R}(e^0) = o(t); \quad h_1, h_2 \in H_u \times H_\alpha; t \in \Lambda.\end{aligned}\right\} \tag{43}$$

In such a case, $V\mathbf{R}(e^0;h)$ is denoted by $D\mathbf{R}(e^0;h)$, and $\mathbf{R}(e)$ admits a total G derivative at $e^0 = (u^0, \alpha^0)$. It follows that the relationship

$$D\mathbf{R}(e^0;h) = \mathbf{R}'_u(e^0)h_u + \mathbf{R}'_\alpha(e^0)h_\alpha \tag{44}$$

holds, where $\mathbf{R}'_u(e^0)$ and $\mathbf{R}'_\alpha(e^0)$ are the partial G derivatives at e^0 of $\mathbf{R}(e)$ with respect to u and α.

With the derivation of Eq. (44), the task outlined in guideline (G.1) has been completed, and Eq. (43) gives the necessary and sufficient conditions underlying this completion. Note also that $\mathbf{R}'_u(e^0)$ is linear operator form H_u into H_R, i.e., $\mathbf{R}'_u(e^0) \in \mathscr{L}(H_u(\Omega), H_R(\Omega_R))$. By analogy to the particular case when the response is a functional [cf. Eq. (19) *et seq.* in Ref. 1], it is still convenient to refer to the quantities $\mathbf{R}'_u(e^0)h_u$ and $\mathbf{R}'_\alpha(e^0)h_\alpha$ appearing in Eq. (44) as the "indirect effect term" and the "direct effect term," respectively.

The direct effect term can be evaluated efficiently at this stage. To proceed with the evaluation of the indirect effect term, consider that the orthonormal set $\{\phi_k\}_{k\in K}$, where k runs through an index set K, is an orthonormal basis of $H_R(\Omega_R)$. Then, since $\mathbf{R}'_u(e^0)h_u \in H_R(\Omega_R)$, it follows that

$$\mathbf{R}'_u(e^0)h_u = \sum_{k\in K} \{\mathbf{R}'_u(e^0)h_u, \phi_k\}\phi_k. \tag{45}$$

The notation $\Sigma_{k\in K}$ is used to signify that in the above sum only an at most countable number of elements are different from zero, and the series extended upon the nonzero elements converges unconditionally. According to customary terminology, the functionals $\{\mathbf{R}'_u(e^0)h_u, \phi_k\}$ are called the Fourier coefficients (in this case, of $\mathbf{R}'_u(e^0)h_u$) with respect to the basis $\{\phi_k\}$. These functionals are linear in h_u since $\mathbf{R}(e)$ was required to satisfy the conditions stated in Eq. (43). Thus, the derivation of Eq. (45) has completed the task outlined in guideline (G.2).

To accomplish the task oulined in guideline (G.3), it is first recalled[1] that the adjoint sensitivity formalism for functionals required the indirect effect term to be represented as an inner product of h_u with an appropriately defined vector in H_u [cf. Eq. (20) in Ref. 1]. This indicates that progress can be made here only if each of the functionals in Eq. (45) is expressed as an inner product of h_u with a uniquely defined vector in $H_u(\Omega)$ yet to be determined.

The construction of the aforementioned inner products can readily be accomplished with the help of the operator adjoint to $\mathbf{R}'_u(e^0)$. Since $\mathbf{R}'_u(e^0) \in \mathscr{L}(H_u(\Omega), H_R(\Omega_R))$, and since Hilbert spaces are self-dual, the adjoint of $\mathbf{R}'_u(e^0)$ is the operator $\mathbf{M}(e^0) \in \mathscr{L}(H_R(\Omega_R), H_u(\Omega))$ defined by means of relationship

$$\{\mathbf{R}'_u(e^0)h_u, \phi_k\} = [h_u, \mathbf{M}(e^0)\phi_k], \quad k \in K. \tag{46}$$

The operator $\mathbf{M}(e^0)$ is unique iff $\mathbf{R}'_u(e^0)$ is densely defined.

The adjoint sensitivity formalism for functionals can now be used to construct the adjoint system whose solution will subsequently enable the elimination of unknown values of h_u from the expression of each functional $[h_u, \mathbf{M}(e^0)\phi_k], k \in K$. To construct this system, the necessary and sufficient conditions[1] underlying the validity of Eqs. (21) and (22) must be satisfied. Then, for every vector $z_k \in H_Q, k \in K$, the following relationship holds:

$$\langle z_k, \mathbf{N}'_u(e^0)h_u\rangle = [\mathbf{L}^*(e^0)z_k, h_u] + \{P(h_u;z_k)\}_{\partial\Omega}, \quad k \in K. \tag{47}$$

where $\mathbf{L}^*(e^0)$ is the operator formally adjoint to $\mathbf{N}'_u(e^0)$, and $\{P(h_u;z_k)\}_{\partial\Omega}$ is the associated bilinear form evaluated on $\partial\Omega$. The adjoint boundary conditions which determine the domain of $\mathbf{L}^*(e^0)$ are obtained by requiring that they satisfy criteria analogous to the criteria satisfied by the adjoint boundary conditions given in Eq. (24). From this requirement and from the fact that Eqs. (47) and (23) are formally indentical it follows that the desired adjoint boundary conditions are formally identical to the boundary conditions given in Eq. (24), and can be expressed as

$$\{\mathbf{B}^*(z_k;e^0) - \mathbf{A}^*(e^0)\}_{\partial\Omega} = \mathbf{0}, \quad k \in K. \tag{48}$$

As before [cf. Eq. (25)], selecting the adjoint boundary conditions given in Eq. (48) reduces the bilinear form $\{P(h_u;z_k)\}_{\partial\Omega}$ appearing in Eq. (47) to $\hat{P}(h_\alpha,z_k;e^0)$. In view of this and of Eq. (21), Eq. (47) becomes

$$[\mathbf{L}^*(e^0)z_k,h_u] = \langle z_k, V\mathbf{Q}(\alpha^0;h_\alpha) - \mathbf{N}'_\alpha(e^0)h_\alpha\rangle - \hat{P}(h_\alpha,z_k;e^0), \quad k\in K. \tag{49}$$

Comparing the left-hand side of Eq (49) with the right-hand side of Eq. (46) shows that

$$\mathbf{L}^*(e^0)z_k = \mathbf{M}(e^0)\phi_k, \quad k\in K. \tag{50}$$

This relationship holds uniquely in view of the Riesz representation theorem.[2]

The construction of the desired adjoint system, consisting of Eq. (50) and the boundary conditions given in Eq. (48) has thus been completed. Furthermore, Eqs. (44), (45), (46), (49), and (50) can now be used to obtain the following expression for the sensitivity $D\mathbf{R}(e^0;h)$ of $\mathbf{R}(e)$ at e^0:

$$D\mathbf{R}(e^0;h) = \mathbf{R}'_\alpha(e^0)h_\alpha + \sum_{k\in K}[\langle z_k, V\mathbf{Q}(\alpha^0;h_\alpha) - \mathbf{N}'_\alpha(e^0)h_\alpha\rangle - \hat{P}(h_\alpha,z_k;e^0)]\phi_k. \tag{51}$$

This accomplishes the desired elimination of all unknown values of h_u from the expression giving the sensitivity of $\mathbf{R}(e)$ at e^0. Note that Eq. (51) includes the particular case of functional-type responses. In such a case, the summation $\Sigma_{k\in K}$ would only contain a single term, and the derivations presented in this section would reduce to those presented in Ref. 1.

To evaluate the sensitivity $D\mathbf{R}(e^0;h)$ by means of Eq. (51), it is required to compute as many adjoint functions z_k from Eqs. (48) and (50) as there are nonzero terms in the representation of $\mathbf{R}'_u(e^0)h_u$ given in Eq. (45). Although the linear combination of basis elements ϕ_k given in Eq. (45) may in principle contain infinitely many terms, obviously only a finite number of the corresponding adjoint functions z_k can be calculated in practice. Therefore special attention is required to select the Hilbert space $H_R(\Omega_R)$, a basis $\{\phi_k\}_{k\in K}$, and a notion of convergence to best suit the problem at hand. This selection is guided by the need to represent the indirect effect term $\mathbf{R}'_u(e^0)h_u$ as accurately as possible with the smallest number of basis elements; a related consideration is the viability of deriving bounds and/or asymptotic expressions for the remainder after truncating Eq. (45) to the first few terms.

The theory developed in this section was successfully applied[6] to compute time-dependent sensitivities of a time-dependent temperature response for a reactor thermal-hydraulic sample problem. Modified Legendre polynomials of the time-variable were used as basis elements. Although the series expressing the indirect effect term [cf. Eq. (45)] contained infinitely many terms, the retention of only the first six terms, and consequently the computation of only six adjoint functions, yielded sensitivities within an overall accuracy of 2% over the entire time interval (100 steps).

IV. SUMMARY AND CONCLUSIONS

Concepts of nonliner functional analysis have been recently employed to develop a sensitivity theory[1] for physical problems described by systems of coupled nonlinear equations, with nonlinear functionals as responses. This sensitivity theory has been extended in the present work to include treatment of more complex responses.

Responses that are functionals defined at a critical point of a function $F(u,x,\alpha)$ of the system's state vector and parameters have been considered first. In practice, this critical point may represent any extremum, saddle, or inflexion point of $F(u,x,\alpha)$. It has been shown that changes in the system parameters affect both the numerical value of the response and the critical point itself. Expressions for the sensitivity of the numerical value of the response and for the sensitivity of the critical point have been obtained within the context of the forward sensitivity formalism by directly applying the definition of the G differential. However, since it is expensive to use this formalism to answer all sensitivity questions that might arise in practice, the adjoint sensitivity formalism has been developed to yield alternative expressions for the desired sensitivities. This formalism requires the computation of as many adjoint functions as there are components of the critical point in phase-space, and of one additional adjoint function to evaluate the sensitivity of the numerical value of the response. Once these adjoint functions have been computed, the sensitivities to *all* possible changes in the system parameters can be obtained by simple quadratures. This makes the adjoint sensitivity formalism the most cost-efficient formalism to use whenever possible, although, as has been discussed, the necessary and sufficient conditions underlying its validity are more restrictive than those underlying the validity of the forward sensitivity formalism.

Sensitivity theory has also been extended to include treatment of general operators as responses. It has been shown that here are essentially no conceptual and computational differences between the treatment of operators and the treatment of functionals as responses within the forward sensitivity formalism. However, there is a considerable difference between the treatment of these two types of responses within the adjoint sensitivity formalism. This formalism can be developed only if the h_u dependence of the G differential giving the sensitivity of the operator-type response is expressible as a linear combination of linear functionals of h_u. For this purpose, it has been necessary and sufficient to consider the response $R(e)$ to be an element of the Hilbert space $H_R(\Omega_R)$, to introduce an orthonormal basis for $H_R(\Omega_R)$, and to require the existence of the G derivative of $R(e)$ at e^0. The indirect effect term has then been expressed as a linear combination of basis elements, each of these elements being multiplied by a linear functional of h_u which contained the entire h_u dependence of the response sensitivity. This h_u dependence has in turn been eliminated from the expression of each of these functionals by using adjoint functions satisfying appropriately constructed adjoint systems.

When derived via the adjoint sensitivity formalism, the exact expression of the sensitivity of an operator-type response contains as many adjoint functions as these are nonzero terms in the linear combination of basis elements [viz., Eq. (45)]. This linear combination may, in principle, contain

infinitely many terms. To minimize the computation of adjoint functions, it becomes important to select a basis and a notion of convergence to represent the indirect effect term as accurately as possible with the smallest number of basis elements. It is also desirable to derive, if possible, bounds and/or asymptotic expressions for the remainder after truncating the linear combination expressing the indirect effect term.

It has already been established (in many works on sensitivity analysis) that the adjoint sensitivity formalism is the most economical to use, whenever possible, if the physical problem involves a large data base (or many alterations in the data) and comparatively few functional-type responses. As the results of this work indicate, this is still the case when the response is a functional defined at a critical point. For operator-type responses, however, the specific needs of sensitivity analysis, the number of system parameters and responses and the characteristics of each response must be examined to determine whether computational costs warrant the use of the adjoint sensitivity formalism.

The theoretical advances which this work contributes to sensitivity theory were made possible by the use of concepts of nonlinear functional analysis. Nonetheless, the potential of using such concepts to extend further the scope of sensitivity theory warrants more research. Present research is divided between developing sensitivity theory and applying existing theory to new areas. The new areas of application include coupled neutronic/thermal-hydraulic problems in reactor safety analysis, problems involving phase changes, and climatic projections based on general circulation models of the atmosphere. An important but presently open question regarding the theory is the effect of the higher-order G differentials of the response. Even if expressions for the higher-order G differentials could be derived, their computation may be prohibitively expensive in practice. Thus, rather than attempt to compute succesively higher order G differentials, it is more useful to derive sharp bounds for their cummulative effect. The possibility of using concepts of nonlinear functional analysis to derive such bounds is currently being researched. The incorporation of these bounds into an uncertainty analysis formalism would result in a reliable and efficient tool for comprehensive sensitivity and uncertainty analyses of complex physical problems.

ACKNOWLEDGMENTS

This work would not have been possible without the strong support of J. Naser of the Electric Power Research Institute, and of C. R. Weisbin and F. C. Maienschein of Oak Ridge National Laboratory (ORNL) Engineering Physics Division. Stimulating discussion with M. C. G. Hall of ORNL are gratefully acknowledged. Special thanks are due to Patty Boit for her expert typing of this paper.

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Resonance poles and Gamow vectors in the rigged Hilbert space formulation of quantum mechanics

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(Received 28 May 1980; accepted for publication 8 May 1981)

After a summary of the rigged Hilbert space formulation of quantum mechanics and a brief statement of its advantages over von Neumann's formulation, a mathematically correct definition of Gamow's exponentially decaying vectors as generalized energy eigenvectors is suggested. It is shown that exponentially decaying vectors are obtained from the S-matrix poles in the lower half of the second sheet and exponentially growing vectors from the S-matrix poles in the upper half of the second sheet. Decaying "state" vectors are defined as functionals over half of the space of physical states and growing "state" vectors are defined as functionals over the other half. On functionals over these subspaces, the dynamical group of time development splits into two semigroups, one for $t > 0$ and the other for $t < 0$. The generalized basis system connected with the spectrum of the Hamiltonian is transformed into a new basis system in which the exponentially decaying component of the density matrix is separated.

PACS numbers: 03.65.Ca, 23.60. + e, 11.20. − e

1. INTRODUCTION

The description of decay phenomena with complex energy eignenfunctions with eigenvalue $E_R - i\Gamma/2$, $\Gamma > 0$, is almost as old as quantum mechanics.[1] But, like plane waves, these decaying wave functions were not considered respectable objects. In the meantime "Dirac states" (kets) have become mathematically well defined objects[2] and are invaluable for the description of scattering states.[3] "Gamow states" for decaying objects are slightly more disreputable: Whereas plane waves—though not elements of Hilbert space—have at least a finite probability density at every point in space, the probability density for the complex energy eigenfunctions diverges as $r \to \infty$. The origin of this "exponential catastrophe" lies in the unphysical assumption that the complex energy eigenfunction describes the decaying state for all time. To eliminate this exponential catastrophe one has to take into account that the decaying state was produced in a scattering process at or before a finite time, say $t = 0$. The decaying state is, therefore, only to be considered for $t > 0$. At earlier times $t < 0$, the system was in a growing state, described by a complex energy eigenfunction with eigenvalue $E_R + i\Gamma/2$. Thus, unlike planes waves, complex energy eigenfunctions have to be separated into two classes, those which are associated with physical states for earlier times and those that are associated with physical states for later times.

For this reason another description was suggested, in which decaying states are not eigenstates but nonstationary states corresponding to the Cauchy problem of the Schrödinger equation.[4] This restricted the description in a natural way to the later times $t \geqslant 0$. But it also led to the shocking observation that these states cannot decay exponentially.[5]

An alternative approach started from the idea that decaying states are almost bound states that come from the discrete eigenvalues in the continuous spectrum of the unperturbed Hamiltonian $H - V$, where V is the decay interaction.[6] This led to the Breit–Wigner energy distribution[7] and the Siegert pole[8] for a resonance. A resonance was defined as a sharp structure in the cross section of an energy E_R where the phase shift $\delta_l(E)$ increased rapidly by π. In the S-matrix theory, decaying states were proposed[9] to be associated with poles in the fourth quadrant of the complex-momentum plane (below the real axis on the second sheet of the energy plane) and growing states with poles in the third quadrant (above the real axis on the second sheet of the energy plane). Due to the mathematical problems connected with the complex energy eigenfunctions, these singularities of the continuation of the S matrix or, somehow related to it, of an appropriate family of matrix elements of the resolvent $(\bar{H} - z)^{-1}$, are most frequently taken as the starting point for the mathematical treatment of resonances.[10] The Wigner–Weisskopf model[6–8] is then the approximation in which all branch cuts are ignored in the evaluation of the decay amplitude and only the pole singularity is retained and put on the first sheet. This approximation destroys the self-adjointness of the Hamiltonian and was thus the first of many assaults upon the self-adjointness,[11] of which the dilatation analytic method is the most promiment.[12] It relates the poles of the resolvent to isolated eigenvalues of a suitable nonself-adjoint analytic continuation of the Hamiltonian. The complementary approach keeps the Hamiltonian self–adjoint and uses analytically continued eigenvectors: Realizing that the poles of the resolvent can be considered as generalized eigenvalues of the Hamilitonian,[13] the corresponding generalized eigenvectors in a suitably defined Rigged Hilbert space were chosen as "quasistationary state vectors."[14]

A third approach towards decaying state vectors started from the definition of a quasistationary state as the intermediate state in a scattering experiment at an energy E_R at which the time delay $t_D^{(E)} = 2[d\delta_l(E)/dE]$ has a sharp maximum—indicating the formation of a projectile—target bound state.[3,15] As a consequence of causality this quasistationary state and the resonance can be shown to be one and the same phenomenon, which is characterized by two num-

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bers: E_R and

$$\Gamma = \left[-2\left(\frac{d\delta_l(E)}{dE} \Big/ \frac{d^3\delta_l(E)}{dE^3} \right)_{E=E_R} \right]^{1/2}.$$

Therefore, starting from the Breit–Wigner energy distribution, a decaying state vector in the Wigner–Weisskopf approximation was introduced[3,16] as the generalized eigenvector of the Hamiltonian with eigenvalue $E_R - i\Gamma/2$ and an expontial time development. For small width (Born appromation) this "Gamow state" led to the Fermi Golden Rule. Combined with analytic continuation techniques this idea was used[17] to separate an exponentially decaying term from the background in the framework of the Friedrichs model.[10]

A resonance and therewith a quasistationary state is always associated with a *pair* of poles in the second sheet of the S matrix, one immediately below the positive real energy axis at $E_R - i\Gamma/2$ and one immediately above the positive real axis at $E_R + i\Gamma/2$. And one can even derive the one-to-one correspondence between the pair of poles and the quasistationary state[3] if one excludes the unlikely case that the fourth and higher derivatives of the phase shift $\delta_l(E)$ are rapidly varying functions.[18] Therefore, "quasistationary state vectors" should also be obtainable from the complex poles of the S matrix. This "Gamow state vector" was the only missing link in the correspondence scheme:

	S-matrix description	Vector space description
Stationary state	Pole on the negative real axis	Eigenvector of H
Scattering state	Cut along the spectrum of $\overline{H}$	Generalized eigenvector of H Dirac-ket
Quasistationary state	Pole in the second sheet	Gamow vector

From the required separation into earlier and later times, which was mentioned at the beginning, we cannot expect that the "Gamow vectors" be like the Dirac ket functionals on the entire space of physical states. Gamow states must be considered separately on the subspaces of earlier and later physical states, the later being related to the Cauchy problem of the Fock–Krylov picture.

The Gamow vectors will be obtained by a transformation from the generalized eigenvector decomposition with respect to the continuous spectrum of H [Eqs. (2.1) or (4.1) below] into a pair of new generalized eigenvector decompositions [Eqs. (3.14) and (3.14′)], in which the contribution from the resonance pole is explicitly contained as one of the generalized basis vectors. This generalized eigenvector obtained from the resonance pole in the lower (upper) second sheet is the decaying (growing) Gamow state vector with exponential time development. It represents the resonance *per se* (characterized by two real parameters) and is independent of the preparation process. A physical decaying state is prepared in a scattering experiment and contains in addition to the reasonance term a background term which depends upon the particular process by which the decaying state was created. This background term is the remainder of the new generalized eigenvector decomposition for a physical decaying state. It is this background term that gives rise to the deviation from the exponential decay law.[5] The analogous observation, that the decay law of an unstable particle depends upon the reaction in which it was created but that the exponentially decreasing term is independent of the preparation, has already been made before in terms of the decay amplitude in the Fock–Krylov picture.[19] This settles the controversy about the memory effects of unstable particles: The geniuine resonance "state" (pole part) decays exponentially; memory effects are due to the background and come from the preparation.

A transformation from the continuous energy representations of the density matrix into a new representation in which the exponentially decaying part is separated has already been suggested by the Brussels group[20] and was to be performed by a nonunitary operator. It cannot be obtained in the Hilbert space framework, as it is defined by a transformation from one generalized basis system into another generalized basis system. The Rigged Hilbert space[2] with a suitably defined topology can accomplish it.

Though the problems treated here could be as well discussed in the conventional von Nuemann formulation of quantum mechanics, the more natural frame is the rigged Hilbert space (RHS) formulation of quantum mechanics.

We will, therefore, first give a brief description of the RHS and the RHS formulation of quantum mechanics in Sec. 2. In Sec. 3 we will show that the second sheet poles below the real energy axis correspond to the exponentially decaying state vectors and the second sheet poles above the real energy axis correspond to the exponentially growing state vectors. In this section it is also shown that the space Φ of physical states for the scattering process in which a resonance occurs contains two subspaces (the sum of which may not be dense in Φ); exponentially growing states are functionals on one and exponentially decaying states are functionals on the other. On the functionals over these subspaces, the dynamical group of time development splits into two semigroups, one for $t < 0$ and one for $t > 0$.

In Sec. 4 an additional assumption about the property of the space of physical states is introduced. Under this assumption the background term takes the form required for the transformation of Ref. 20 and the density matrix can be expressed in a new continuous energy representation with separate exponentially decaying parts.

2. RIGGED HILBERT SPACE AND QUANTUM MECHANICS

A. The rigged Hilbert space

The rigged Hilbert space[2] provides the mathematical tools for a rigorous formulation of the Dirac formalism. According to Dirac,[21] every vector ϕ representing a physical state is expanded with respect to a basis system of eigenvectors of observables:

$$\phi = \int_{\mathrm{Sp}\overline{H}} dE\, |E\rangle\langle E|\phi\rangle, \tag{2.1}$$

where as the observable we have chosen the Hamilton operator H:

$$H|E\rangle = E|E\rangle \tag{2.2}$$

and have ignored—as we will do throughout this paper—any possible degeneracy. $\phi(E) = \langle E|\phi\rangle$ is the well-behaved wavefunction (in the energy representation) and $\mathrm{Sp}\overline{H}$ is the spectrum of H that was identified with the set of possible eigenvalues E in (2.2) which were believed to be real. However, (2.1) is not possible for every $\phi \in$ Hilbert spae $\mathscr{H}$, $|E\rangle$ are in general not elements of $\mathscr{H}$, and (2.2) requires further specifications. These specifications can be chosen such that (2.2) is also valid for complex values of E. The mathematics that justifies (2.1) and specifies (2.2) is given by the rigged Hilber spaces.

To obtain a RHS one takes a linear space Ψ with a scalar product and completes[22] it with respect to two topologies[22] $\tau_{\mathscr{H}}$ and τ_{Φ}. The Hilbert space—or $\tau_{\mathscr{H}}$—convergence is defined by

$$\phi_\nu \overset{\tau_{\mathscr{H}}}{\longrightarrow} \phi \Longleftrightarrow ||\phi_\nu - \phi|| \to 0 \quad \text{for } \nu \to \infty.$$

The τ_ϕ convergence must fulfill certain conditions (nuclearity) and cannot be given by one norm or scalar product but may be given by a countable number of scalar products. It is stronger than $\tau_{\mathscr{H}}$, i.e., from $\phi_\nu \overset{\tau_\phi}{\longrightarrow} \phi$ follows $\phi_\nu \overset{\tau_{\mathscr{H}}}{\longrightarrow} \phi$, but in general not vice versa. Consequently, there are more $\tau_{\mathscr{H}}$-limit points than τ_ϕ-limit points in the completions of Ψ, so that $\Phi \subset \mathscr{H}$ if Φ denotes the linear scalar product space, which is the τ_ϕ-completion, and $\mathscr{H}$ the $\tau_{\mathscr{H}}$ completion of Ψ.

The conjugate space $\mathscr{H}^\times$ and $\Phi^\times$ are spaces of $\tau_{\mathscr{H}}$- and τ_Φ-continuous *anti*linear functionals, respectively. A continuous antilinear functional is a function, F, on a linear space, written $F(\phi) = \langle \phi|F\rangle$, that satisfies

(1) $\langle \alpha\phi + \beta\psi|F\rangle = \bar{\alpha}\langle\phi|F\rangle + \bar{\beta}\langle\psi|F\rangle$ (antilinearity) for $\phi,\psi \in$ space; $\alpha,\beta \in \mathbb{C} =$ complex numbers.

(2) From $\phi_\nu \overset{\tau}{\longrightarrow} \phi$ follows $\langle\phi_\nu|F\rangle \overset{\tau_{\mathbb{C}}}{\longrightarrow} \langle\phi|F\rangle$, where τ is the topology of the linear space (i.e.), either τ_Φ or $\tau_{\mathscr{H}}$ and $\tau_{\mathbb{C}}$ is the usual topology of the complex numbers.

As condition (2) is more stringent for $\tau_{\mathscr{H}}$ than for τ_ϕ (there are more $\tau_{\mathscr{H}}$-limit points than τ_ϕ-limit points), it follows that $H^\times \subset \Phi^\times$. Further, for every $\tau_{\mathscr{H}}$-continuous functional $\langle\phi|F^{(\mathscr{H})}\rangle$, there exists an $f \in \mathscr{H}$ such that $\langle\phi|F\rangle = (\phi, f)$, where (ϕ, f) denotes the scalar product (Frechet–Riesz theorem). Therefore, one can identify $\mathscr{H}^\times$ with $\mathscr{H}$ by equating $F^{\mathscr{H}} = f \in \mathscr{H}$ and obtain

$$\Phi \subset \mathscr{H} \subset \Phi^\times \tag{2.3}$$

This trinity of spaces is the RHS. The Dirac bracket $\langle\phi|F\rangle$ is then the extension of the scalar product (ϕ, f) for those $F \in \Phi^\times$ which are not in $\mathscr{H}$. Φ is always reflexive, $\Phi^{\times\times} = \Phi$, and the functional $\tilde{\phi}(F)$ on $\Phi^\times$ is $\langle F|\tilde{\phi}\rangle = \overline{\langle\phi|F\rangle}$.

To the triplet of spaces (2.3) corresponds for every observable a triplet of linear operators

$$A \subset \overline{A} \subset A^\times. \tag{2.4}$$

For A we always choose continuous (= bounded) operators in Φ and the closure $\overline{A}$ of A is in general not a continuous Hilbert space operator. The conjugate operator $A^\times$ in $\Phi^\times$, which is continuous but in general not bounded is defined by

$$\langle\phi|A^\times|F\rangle = \langle A\phi|F\rangle \quad \phi \in \Phi, \quad F \in \Phi^\times. \tag{2.5}$$

Generalized eigenvectors F_ω of A with eigenvalue ω are defined by

$$\langle\phi|A^\times|F_\omega\rangle = \langle A\phi|F_\omega\rangle = \omega\langle\phi|F_\omega\rangle \quad \text{for every } \phi \in \Phi, \tag{2.6}$$

which is also written as

$$A^\times|\omega\rangle = \omega|\omega\rangle \quad \text{or simply } A|\omega\rangle = \omega|\omega\rangle, \tag{2.6'}$$

denoting the triplet (2.4) just by the one symbol A. Equation (2.6) gives a precise meaning to (2.2) if the RHS (2.3) has been completely specified. The set of possible values for ω (the set of generalized eigenvalues) depends upon the choice of Φ. Above we have only said that Φ is a nuclear linear topological space (with the topology perhaps given by a countable, but not finite, number of scalar products) but have not completely specified it. The particular choice of Φ depends upon the particular physical system that one wants to describe.[23]

For an essentially self-adjoint (esa) H, i.e., an operator whose Hilbert space adjoint $H^\dagger = \overline{H}$, there exists always a sufficient set of generalized eigenvectors. i.e., there exists $|E\rangle$ such that every $\phi \in \Phi$ (but not every $h \in \mathscr{H}$) can be written in the form (2.1). This is called the nuclear spectral theorem or the Dirac spectral theorem, because it justifies Dirac's hypothesis (2.1) and makes it precise. Though, according to this theorem, there is always a sufficient set of $|E\rangle$, the set of $|E\rangle$ that occurs in (2.1) does in general not exhaust[24] the set of $|E\rangle$ which fulfills (2.2). And there are in general more generalized eigenvalues E of H than belong to $\mathrm{Sp}\overline{H}$. In particular, for an essentially self-adjoint operator H for which $\mathrm{Sp}\overline{H}$ is real, there can exist complex generalized eigenvalues, and instead of the integral over $\mathrm{Sp}\overline{H}$ in (2.1) one may have an integral over a contour in the complex plane, as we shall discuss below. What set of generalized eigenvalues E in (2.2) are allowed depends on the particular choice of Φ; conversely, one may specify Φ by specifying the analyticity property of the complex extension of the wavefunction $\phi(E) = \langle E|\phi\rangle$.

B. The RHS formulation of quantum mechanics

von Neumann's Hilbert space (H.S) formulation of quantum mechanics[25,26] assumes the one-to-one correspondence between (pure) physical states and elements (rays) of the Hilbert space $\mathscr{H}$ and between physical observables and linear (Hermitian) operators of $\mathscr{H}$. This is a mathematical utopianization which cannot be justified by physical arguments,[27–30] since up to an arbitrary small error of the measurements one can always approximate any element of $\mathscr{H}$ by an element of a dense linear subspace. Instead of using the $\tau_{\mathscr{H}}$-completion for the space of (pure) physical states one could also use the τ_Φ-completion. This leads to the (RHS) formulation of quantum mechanics. It is again a mathematical utopianization which, however, is mathematically more convenient and provides a much more natural description of the physical phenomena.

Whereas in (the contemporary version of)[26] the HS formulation of quantum mechanics each kind of microsystem

(like, e.g., electrons or hydrogen atoms or CO molecules) has as the space of physical states a Hilbert space $\mathscr{H}$, in the RHS fromulation[31,32,...,35] the space of physical preparable states of one kind of systems is given by a nuclear space Φ, which is $\tau_\mathscr{H}$-dense in $\mathscr{H}$. The choice of the nuclear topology is determined by mathematical convenience and is different for different kinds of microsystems (see Refs. 23 and 27).

The scattering states (generalized eigenvectors of the continuous spectrum) and the decaying states (complex energy eigenvectors) can already be made mathematically rigorous if one uses the RHS in von Neumann's formulation of quantum mechanics. But the full benefit of the RHS can only be realized in the RHS formulation of quantum mechanics.

The RHS formulation has the following advantages over the conventional HS formulation.

1. Some $\tau_\mathscr{H}$-limit elements, like states with infinite energy (Hilbert space vectors which are not in the domain of the energy operator), are not τ_ϕ-limit elements. This excludes the infinite energy states from the space of physical states Φ in the RHS formulation.

2. The wavefunction $\phi(E) = \langle E|\phi\rangle$ is a well behaved continuous infinitely differentiable function (element of the Schwartz space) in the RHS formulation, whereas in the HS formulation the wave function $h(E)$ of one particular state $h \in \mathscr{H}$ is given by any element of a set $\{h(E)\}$ of Lebesque square integrable functions which differ on a set of measure zero. The modulus square of the wavefunction characterizes the appartus resolution of the experiment by which the state was prepared and a Schwartz space function gives a description much closer to the experimentally detectable situation than a set of Lebesque square integrable functions.

3. The algebra of observables $\mathscr{A}$ for perhaps all physical systems can be represented by an algebra of continuous operators in Φ, whereas already the simplest algebra of observables—the algebra generated by P,Q, 1 fulfilling $[P,Q] = -i1$—must be represented by unbounded operators in $\mathscr{H}$. This avoids in the RHS formulation all problems with the domain of definition of an observable.

4. Every Hermitian (esa) observable has a complete set of generalized eigenvectors in $\Phi^\times$, and every physically preparable state $\phi \in \Phi$ can be expanded with respect to this generalized basis system according to (1). In the HS formalism this distinction between physically preparable states and idealized scattering states does not exist, as scattering states do not exist in $\mathscr{H}$. Though such idealized monochromatic states cannot be physically prepared, their use simplifies the calculations and is always possible when the resolution of the apparatus is sharper than structures of the physical system.[36]

With advantages 3 and 4 one has recovered the Dirac formalism in a mathematically rigorous form and these points were the original motivation for the RHS formulation[31,32]; the following advantages came as a bonus:

5. Decaying and growing states, defined by pairs of complex poles of the S matrix (or resolvent of $\overline{H}$), can be described by generalized eigenvectors of H (i.e., $\in\Phi^\times$) with complex eigenvalues.

Instead of (1), $\phi\in\Phi$ can be expanded with respect to a generalized basis system that contains the exponentially decaying or growing "state" vector. It is this last point that we wish to discuss in the following section.

3. DECAYING AND GROWING GAMOW STATE VECTORS AND THEIR ASSOCIATION TO THE RESONANCE POLES OF THE S MATRIX

A. Deforming the contour of integration to separate the pole term

We now want to derive the Gamow state vectors from the resonance poles of the S matrix. This can be done analogously to the extraction of the bound state vector from the bound state pole of the S matrix.[37] We write the S-matrix element at any time t (it is independent of t) as

$$(\psi^{\text{out}}(t), S\psi^{\text{in}}(t)) = (\Omega^-\psi^{\text{out}}(t), \Omega^+\phi^{\text{in}}(t)) = (\psi^-(t), \phi^+(t))$$
$$= \int_{\overline{\text{Sp}}\,\overline{H}} dE' \langle\psi^-|E'^-\rangle S(E')\langle{}^+E'|\phi^+\rangle. \quad (3.1)$$

The notation here is the conventional one[38]:

$$|E^\pm\rangle = |E\rangle + \frac{1}{E - H \pm i0} V|E\rangle = \Omega^\pm|E\rangle,$$

where

$$(H - V)|E\rangle = E|E\rangle$$

(Lippman–Schwinger equation), Ω^+ and Ω^- are the Møller wave operators, $\phi^+(t)$ represents the state that develops from the prepared in-state ϕ^{in}; $\psi^-(t)$ represents the state that develops into the measured out-state ψ^{out}.

$$\left.\begin{matrix}\langle{}^+E|\phi^+\rangle = \langle E|\phi^{\text{in}}\rangle \\ \langle{}^-E|\psi^-\rangle = \langle E|\psi^{\text{out}}\rangle\end{matrix}\right\} \text{are the energy wave functions} \quad (3.2)$$

representing the energy distribution on the

$$\left\{\begin{matrix}\text{prepared state } \phi^{\text{in}} \\ \text{measured state } \psi^{\text{out}}\end{matrix}\right\},$$

$|\langle E|\phi^{\text{in}}\rangle|^2$ is given by the incident beam resolution and $|\langle E|\psi^{\text{out}}\rangle|^2$ is measured by the (ideal) detector.

$$\phi^+ = \phi^+(t=0),\ \phi^+(t) = e^{-iHt}\phi^+,\ \phi^{\text{in}}(t) = e^{-i(H-V)t}\phi^{\text{in}},$$
$$\psi = \psi^-(t=0),\ \psi^-(t) = e^{-iHt}\psi^-,\ \psi^{\text{out}}(t) = e^{-i(H-V)t}\psi^{\text{out}} \quad (3.3)$$

The integration in (3.1) is along the upper rim of the cut of the physical sheet for the S matrix $S(E)$ (indicated by $\overline{\text{Sp}}\,\overline{H}$). All extra quantum numbers besides the energy are ignored.

As we are only interested in the principle that establishes the connection between resonance poles and the Gamow state vectors and do not want to burden ourselves with irrelevant details, we will restrict ourselves to a rather uncomplicated physical system. We assume that our model system is, among others, characterized by an S-matrix element (one particular partial wave and all other quantum numbers fixed and ignored) which has the property:

The analytically continued S matrix $S(\omega)$, where ω is the complex energy variable, has no other singularity off the real axis but one pair of poles at $\omega = z_R$ and $\omega = z_R^*$ with $z_R = E_R - i\Gamma/2$, $\Gamma > 0$. The spectrum of $\overline{H}$ is the positive real line.[39] (3.4)

We will also assume of our paradigm system that:

The product of wavefunction and S matrix vanishes on

the lower and upper infinite semicircle on the second sheet.[39] (3.5)

Whereas requirements (3.4) and (3.5) are no cause for worry, we have no proof yet that the following requirements are not too strong. Nevertheless we believe that for reasonable physical systems we can make the following requirements:

The space of physical states Φ is such that the analytically continued wavefunctions[40]

$$\langle \omega^* | \phi^{\text{in}} \rangle = \langle {}^+\omega^* | \phi^+ \rangle = \langle \phi^+ | \omega^+ \rangle^*$$

and

$$\langle \psi^{\text{out}} | \omega \rangle = \langle \psi^- | \omega^- \rangle \tag{3.6a}$$

are analytic functions in the lower half second sheet.

These analytic functions vanish sufficiently fast at the lower infinite semicircle of the second sheet. (3.6b)

The precise formulation of the requirement (3.6b) will be given in the derivation below.

With these requirements the analytically continued integrant in (3.1) has as the only singularity in the lower half second sheet the pole at $\omega = z_R = E_R - i\Gamma/2$. The path of integration of (3.1) can then be easily deformed from the upper rim along the cut into the lower half plane of the second sheet, and (3.1) can be written as

$$(\psi^-(t), \phi^+(t)) = \int_{\mathscr{C}_-} d\omega \langle \psi^- | \omega^- \rangle S_{\text{II}}(\omega) \langle {}^+\omega^* | \phi^+ \rangle + \int_{\circlearrowright} d\omega \langle \psi^- | \omega^- \rangle \frac{\mathscr{s}_{-1}}{\omega - z_R} \langle {}^1\omega^* | \phi^+ \rangle, \tag{3.7}$$

where $\mathscr{s}_{-1}$ is the residium of $S(\omega)$ in the second sheet at z_R:

$$S_{\text{II}}(\omega) = \frac{\mathscr{s}_{-1}}{\omega - z_R} + \mathscr{s}_0 + \mathscr{s}_1(\omega - z_R) + \cdots \tag{3.8}$$

and $\mathscr{C}_-$ is the path below the pole at z_R and $\circlearrowright$ is the circular path around z_R as shown in Fig. 1(a).

If (3.5) and (3.6b) are fulfilled, then the contour $\mathscr{C}_-$ can be deformed into a contour along the negative real axis and along the lower infinite semicircle and the integral along the latter is zero. The path $\circlearrowright$ of the second integral in (3.7) can be deformed into the infinite semicircle (along which the integral vanishes) and the real line from $-\infty$ to $+\infty$. Then (3.7) can be written

$$(\psi^-, \phi^+) = \text{background} + \int_{-\infty_{\text{II}}}^{+\infty} dE' \langle \psi^- | E'_{\text{II}} - i\epsilon \rangle \frac{\mathscr{s}_{-1}}{E'_{\text{II}} - i\epsilon - z_R} \langle {}^+E'_{\text{II}} - i\epsilon | \phi^+ \rangle, \tag{3.9}$$

where we have denoted, for reasons that will become clear later;

$$\text{background} = \int_0^{-\infty_{\text{II}}} dE' \langle \psi^- | E'_{\text{II}} - i\epsilon^- \rangle S(E'_{\text{II}} - i\epsilon) \langle {}^+E'_{\text{II}} - i\epsilon | \phi^+ \rangle. \tag{3.10}$$

The wavefunctions that occur in (3.9) and (3.10) for negative nonphysical values of E are obtained from the physical values by suitable analytic continuation. The integrals in (3.9) and (3.10) run along the negative real axis[41] in the second sheet and along the upper rim of the cut from 0 to ∞ on the physical sheet (or on the lower rim of the cut form 0 to ∞ on the second sheet).

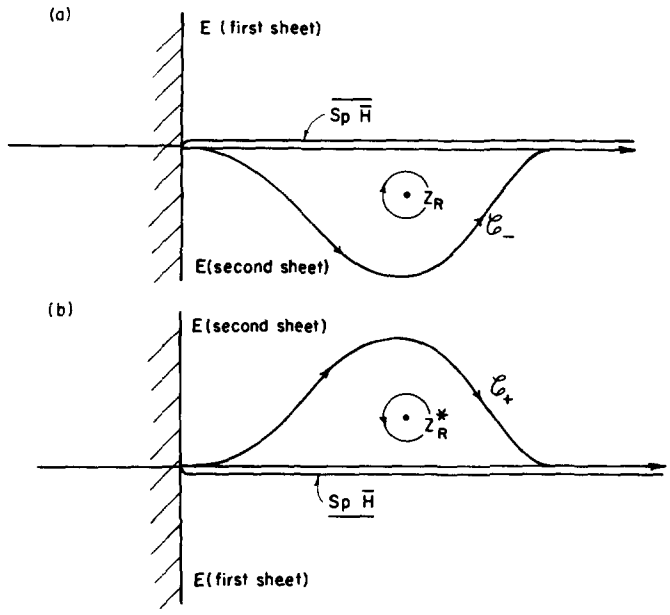

FIG. 1. Deformation of the path of integration into the second sheet of the energy plane. Part (a) is for the decaying state, (b) for the growing state.

The complement of the requirement (3.6) is the following requirement:

The space of physical states ϕ is such that the analytically continued wavefunctions

$$\langle \omega^* | \psi^{\text{out}} \rangle = \langle {}^-\omega^* | \psi^- \rangle = \langle \psi^- | \omega^- \rangle^*$$

and

$$\langle \phi^{\text{in}} | \omega \rangle = \langle \phi^+ | \omega^+ \rangle \tag{3.6a'}$$

are analytic functions in the upper half second sheet.

These analytic functions vanish sufficiently fast at the upper infinite semicircle of the second sheet. (3.6b')

We will now discuss the two cases in which we make use of (3.6) or (3.6') separately and label the corresponding equations by unprimed or primed numbers, respectively. (Note that the same symbols ψ^-, ϕ^+ will have different meanings for the primed and unprimed equations which describe two entirely unrelated problems for the same S matrix.)

With assumptions (3.4), (3.5) and (3.6) the analytically continued integrand in (3.1) has as the only singularity in the upper half second sheet the pole at $\omega = z_R^* = E_R + i\Gamma/2$. In order to deform the path of integration into the upper half second sheet we have to take the complex conjugate of (3.1) and use the symmetry relation of the S matrix.[42]

$$S^*(E + i\epsilon) = S(E - i\epsilon).$$

Then (1) is written

$$(\phi^+, \psi^-) = \int_{\text{Sp}\bar{H}} dE \langle \phi^+ | E^+ \rangle S(E) \langle {}^-E | \psi^- \rangle, \tag{3.1'}$$

where the integration runs now along the lower rim of the cut in the physical sheet (indicated by Sp$\bar{H}$). The path of integration can then easily be deformed into the upper half

second sheet and (3.1′) can be written

$$(\phi^+(t),\psi^-(t)) = \int_{\mathscr{C}_+} d\omega \langle \phi^+|\omega^+\rangle S_{II}(\omega)\,\langle {}^-\omega^*|\psi^-\rangle + \int_{\mathsf{C}} d\omega \langle \phi^+|\omega^+\rangle \frac{s_{-1}}{\omega - z_R^*\langle {}^-\omega^*|\psi^-\rangle}, \quad (3.7')$$

where s_{-1} is the residium of $S(\omega)$ in the second sheet at z_R^*,:

$$S_{II}(\omega) = \frac{s_{-1}}{\omega - z_R^*} + s_0 + s_1(\omega - z_R^*) + \cdots \quad (3.8')$$

and $\mathscr{C}_+$ is the path above the pole at z_R^* and C is the circular path around z_R^* as shown in Fig. 1(b). Again assuming sufficiently nice properties of $\langle \phi^+|\omega^+\rangle$, $\langle {}^-\omega^*|\psi^-\rangle$ and $S(\omega)$ this can be written

$$(\phi^+,\psi^-) = \text{background} + \int_{-\infty_{II}}^{+\infty} dE\,\langle \phi^+|E_{II}+i\epsilon^+\rangle \frac{s_{-1}}{E_{II}+i\epsilon - z_R^*}\langle {}^-E_{II}+i\epsilon|\psi^-\rangle, \quad (3.9')$$

where

$$\text{background} = \int_0^{-\infty_{II}} dE\,\langle \phi^+|E_{II}+i\epsilon^+\rangle S(E_{II}+i\epsilon)\langle {}^-E_{II}+i\epsilon|\psi^-\rangle. \quad (3.10')$$

The integrals in (3.9′) and (3.10′) run along the negative real axis in the second sheet[41] and along the lower rim of the cut from 0 to ∞ on the physical sheet (or on the upper rim of the cut from 0 to ∞ on the second sheet).

The second integral in (3.7) and (3.7′) give, by the Cauchy integral formula,

$$-2\pi i s_{-1}\langle \psi^-|z_R^-\rangle\,\langle {}^+z_R|\phi^+\rangle \quad (3.11)$$

and

$$2\pi i s_{-1}\langle \phi^+|z_R^*\rangle\,\langle {}^-z_R^*|\psi^-\rangle, \quad (3.11')$$

respectively. For this only the properties (3.6a) and (3.6a′) are required.

Equations (3.11) and (3.11′) are the expressions that we wish to obtain but we want to relate them to the second integral in (3.9) and (3.9′), as these have the characteristic Breit–Wigner denumerator. For this the requirements (3.6b) and (3.6b′) are needed in the precise form

$$\langle \psi^-|E^-\rangle\langle {}^+E|\phi^+\rangle \in L^p_-(E_{II}) \quad (3.6)$$

and

$$\langle \phi^+|E^+\rangle\langle {}^-E|\psi^-\rangle \in L^p_+(E_{II}), \quad (3.6')$$

where $1 \leqslant p < \infty$, and where $L^p_\pm(E)$ denotes the space of $\mathfrak{H}^p$ functions[43] with respect to the upper (+) and lower (−) plane of the *second* sheet. The equalities of (3.11) and (3.11′) [i.e., the second integrals of (3.7) and (3.7′)] and the second integrals of (3.9) and (3.9′) follow then from a general theorem [44] (generalization of the Titchmarsh theorem [45]).

We will make the weakest of the requirements (3.6) and (3.6′) $p = 1$, because these hold if

$$\langle \psi^-|E^-\rangle \in L^2_-(E_{II}), \quad (3.12)$$

$$\langle \phi^+|E^+\rangle \in L^2_+(E_{II}). \quad (3.12')$$

As $\psi^-, \phi^+ \in \Phi$ and not only $\in \mathscr{H}$, and the operators H^q ($q = 0,1,2,\ldots$) are τ_Φ-continuous, it follows that not only (3.12) and (3.12′) hold but also that

$$E^q\langle \psi^-|E^-\rangle \in L^2_-(E_{II}), \quad (3.12a)$$

$$E^q\langle \phi^+|E^+\rangle \in L^2_+(E_{II}), \quad (3.12a')$$

Thus the wavefunctions

$$\langle E|\psi^{out}\rangle = \langle {}^-E|\psi^-\rangle = \langle \psi^-|E^-\rangle^* \in L^2_+(E_{II}) \quad (3.13)$$

and

$$\langle E|\phi^{in}\rangle = \langle {}^+E|\phi^+\rangle = \langle \phi^+|E^+\rangle^* \in L^2_-(E_{II}) \quad (3.13')$$

are well behaved Hardy class functions with respect to the upper and lower half-plane of the physical sheet for the case (3.6) and (3.6′), respectively. This we write as

$$\psi^- \in \mathscr{H}_+, \quad (3.13a)$$

$$\phi^+ \in \mathscr{H}_- \quad (3.13a')$$

where $\mathscr{H}_+(\mathscr{H}_-)$ is the Hilbert space which is realized by the space of wavefunctions $\langle {}^-E|\psi^-\rangle(\langle {}^+E|\phi^+\rangle)$.

B. The vector with exponential time development

It is now already obvious that the pole terms, i.e., the second integrals in (3.9) and (3.9′), will be the starting point for the definition of decaying and growing state vectors, respectively. We will now show that this is indeed the case and that we have for the second term in (3.9) an exponential time development, but only for $t > 0$. For the second term in (3.9′) we also have an exponential time development; this, however, is valid only for $t < 0$. In the following Sec. 3C we will show that this separation into processes for $t < 0$ and $t > 0$ is completely natural and exactly as one expects from the intuitive requirements for a formation and decay process, respectively.

We insert (3.11) and (3.10) into (3.9) and omit the arbitrary $\psi^- \in \mathscr{H}_+ \cap \Phi$, then we obtain the representation of ϕ^+:

$$\phi^+ = \int_0^{-\infty_{II}} dE\,|E^-\rangle S_{II}(E)\langle {}^+E|\phi^+\rangle + |z_R^-\rangle(-2\pi i s_{-1})\langle {}^+z_R|\phi^+\rangle, \quad (3.14)$$

where the vector $|z_R^-\rangle$ is defined by

$$|z_R^-\rangle = -\frac{1}{2\pi i}\int_{-\infty}^{+\infty} dE\,|E^-\rangle \frac{1}{E - z_R} \quad (3.15)$$

(integrated along the lower rim of the real axis in the second sheet). (3.15)

We emphasize tht (3.14) is only valid when considered as a functional over $\mathscr{H}_+ \cap \Phi$, and $|z_R^-\rangle$ of (3.15) is therefore only defined as a functional over $\mathscr{H}_+ \cap \Phi$.

Analogously we insert (3.11′) and (3.10′) into (3.9′) and omit the arbitrary $\phi^+ \in \mathscr{H}_- \cap \Phi$, then we obtain the representation of ψ^-:

$$\psi^- = \int_0^{-\infty_{II}} dE\,|E^+\rangle S_{II}(E)\langle {}^-E|\psi\rangle + |z_R^{*\cdot}\rangle(2\pi i s_{-1})\langle {}^-z_R^*|\psi^-\rangle, \quad (3.14')$$

where the vector $|z_R^{*\cdot}\rangle$ is defined by

$$|z_R^{*\cdot}\rangle = \frac{1}{2\pi i}\int_{-\infty}^{+\infty} dE\,|E^+\rangle \frac{1}{E - z_R^*} \quad (3.15')$$

(integrated along the upper rim of the real axis in the second sheet).

Equation (3.14') is only valid when considered as a functional over $\mathscr{H}_-\cap\Phi$ and $|z_R^{*-}\rangle$ of (3.15') is only defined as a functional over $\mathscr{H}_-\cap\Phi$.

Equation (3.15) is the generalized complex energy eigenvector with Breit–Wigner energy distribution introduced before.[3,16] That the functionals (3.15) and (3.15') are indeed generalized eigenvectors of H, written formally as [46]

$$H|z_R^-\rangle = z_R|z_R^-\rangle \tag{3.16}$$

and

$$H|z_R^{*+}\rangle = z_R^*|z_R^{*+}\rangle, \tag{3.16'}$$

follows from the fact that not only $\langle\psi^-|E^-\rangle \in L^2_-(E)$ and $\langle\phi^+|E^+\rangle \in L^2_+(E)$ but also $\langle\psi^-|E^-\rangle E \in L^2_-(E)$ and $\langle\phi^+|E^+\rangle E \in L^2_+(E)$, so that for these functions also the general theorem [44] can be applied, which led from (3.9) and (3.9') to (3.11) and (3.11').

The functionals (3.15) and (3.15') are also generalized eigenvectors of e^{-iHt} for $t > 0$ and $t < 0$, respectively. But (3.15) is not a generalized eigenvector of e^{-iHt} for $t < 0$ and (3.15') is not a generalized eigenvector of e^{-iHt} for $t > 0$.

This follows from the fact that with (3.12) one has also

$$\langle\psi^-|E^-\rangle e^{-iEt} \in L^2_-(E) \quad \text{for } t > 0 \tag{3.17}$$

and with (3.12') one has also

$$\langle\phi^+|E^+\rangle e^{-iEt} \in L^2_+(E) \quad \text{for } t < 0. \tag{3.17'}$$

Then one considers (3.15) as a functional over $\tilde{\psi}^- \in \mathscr{H}_+\cap\phi$ and obtains

$$\langle\tilde{\psi}^-|e^{-iHt}|z_R^-\rangle = -\frac{1}{2\pi i}\int_{-\infty}^{+\infty} dE\,\langle\tilde{\psi}^-|E^-\rangle\frac{e^{-iEt}}{E-z_R},$$
$$\tilde{\psi}^- \in \mathscr{H}_+\cap\Phi.$$

Because of (3.17) one can apply to the right hand side of this equation for $t > 0$ only the general theorem [44] and obtain

$$\langle\tilde{\psi}^-|e^{-iHt}|z_R^-\rangle = e^{-iz_Rt}\langle\tilde{\psi}^-|z_R^-\rangle.$$

This is formally written as [46]

$$e^{-iHt}|z_R^-\rangle = e^{-iz_Rt}|z_R^-\rangle = e^{-iE_Rt}e^{-(\Gamma/2)t}|z_R^-\rangle$$
$$\text{for } t > 0. \tag{3.18}$$

in an analogous way one shows that[46]

$$e^{-iHt}|z_R^{*+}\rangle = e^{-iz_R^*t}|z_R^{*+}\rangle = e^{-iE_Rt}e^{+(\Gamma/2)t}|z_R^{*+}\rangle$$
$$\text{for } t < 0. \tag{3.18'}$$

Equations (3.17), (3.18) and (3.17'), (3.18') identify the $|z_R^-\rangle$ and $|z_R^{*+}\rangle$ as generalized eigenvectors of the energy operator describing exponentially decaying and exponentially growing "states", respectively. We will therefore call them Gamow vectors. For the decay, t must be larger than the (arbitrarily chosen) time $t = 0$, and for the growth, t must be smaller than zero. As already mentioned we will show below in Sec. 3C that this is connected to a natural intuitive requirement for decaying and growing states, respectively.

How these Gamow vectors avoid the well-known pathologies known as the deviations from the exponential decay law[5,18] is also immediately seen: There is no deviation from the exponential law for large t because the integrals over the energy in (3.15) and (3.15') are not bounded from below. Equations (3.15) and (3.15') have ideal Breit–Wigner energy distributions extending from $-\infty$ to $+\infty$ but in the second sheet. And there is no deviation for small t because the Gamow vectors (3.15) and (3.15') are not in the domain of the Hilbert space operator $\overline{H}$ (the closure of the Hamiltonian). This, however, does not mean that there is no deviation from the exponential time development for a physical state. This deviation is due to the background, as we shall discuss in Sec. 3D.

That the decaying states lead in the Born approximation to the Fermi Golden Rule has already been shown in Ref. 16. There it has also been shown that the generalized eigenvectors $|z_R^-\rangle$ are in a certain sense normalizable, $\langle {}^-z_R^*|z_R^-\rangle = 1/2\pi\Gamma$. One may, therefore, define the normalized Gamow vectors

$$\phi^D = \left|E_R - i\frac{\Gamma^-}{2}\right\rangle = \left|E - i\frac{\Gamma^-}{2}\right\rangle(2\pi\Gamma)^{1/2}\frac{\mathcal{S}_{-1}}{\mathcal{S}_{-1}^*}(-1), \tag{3.20}$$

$$\langle\phi^D| = \langle {}^-z_R^*| = \langle {}^-z_R^*|(2\pi\Gamma)^{1/2}\frac{\mathcal{S}_{-1}^*}{\mathcal{S}_{-1}}(-1) \tag{3.20a}$$

and

$$\psi^G = \left|E_R + i\frac{\Gamma^+}{2}\right\rangle = \left|E + i\frac{\Gamma^+}{2}\right\rangle(2\pi\Gamma)^{1/2}\frac{S_{-1}^*}{S_{-1}}, \tag{3.20'}$$

$$\langle\psi^G| = \langle {}^+z_R| = \langle {}^+z_R|(2\pi\Gamma)^{1/2}\frac{S_{-1}}{S_{-1}^*}. \tag{3.20a'}$$

The time development of ϕ^D is only defined into the foward direction, $t > 0$[46]:

$$\phi^D(t) = e^{-iHt}\phi^D = e^{-iE_Rt}e^{-(\Gamma/2)t}\phi^D \quad t > 0 \tag{3.21}$$

and the time development of ψ^G is only defined from the backward direction, $t < 0$[46]:

$$\psi^G(t) = e^{-iHt}\psi^G = e^{-iE_Rt}e^{(\Gamma/2)t}\psi^G) \quad t < 0. \tag{3.21'}$$

ϕ^D is considered as functional on $\Phi\cap\mathscr{H}_+$ and ψ^G is considered as functional on $\Phi\cap\mathscr{H}_-$. By the separation of the space of physical states into these two subspaces the dynamical group e^{-iHt} has been separated into two dynamical semigroups, as indicated by Eqs. (3.21) and (3.21').

C. Separation of resonance scattering into decay and formation

In Sec. 3A we have seen that in order to relate the second sheet pole of the S matrix below the real axis with the vector (3.15) of the Breit–Wigner energy distribution we had to require that (3.6), (3.12), (3.13), or (3.13a) be fulfilled for the out-states of the scattering process described by this S matrix. Then we saw in Sec. 3B that the exponential time development (3.18) could only be derived for (3.15) over these out-states $\psi^- \in \mathscr{H}_+\cap\Phi$ and only for $t > 0$. Analogously we have seen in Sec. 3A that in order to relate the second sheet pole above the real axis with the vector (3.15') we had to require (3.6'), (3.12'), (3.13'), or (3.13a') for the in-states. And in Sec. 3B we saw that the exponential time de-

velopment (3.18′) could only be derived for (3.15′) over these in-states $\phi^+ \in \mathscr{H}_- \cap \Phi$ and that this holds only for $t < 0$. We will now show that this mathematical condition on the ψ^- in the form (3.12) is related to the intuitive conditions for the later part, $t > 0$, of a resonance scattering process. And we will also show that the mathematical condition on the ϕ^+ in the form (3.12′) is related to the intuitive condition for the earlier part, $t < 0$, of a resonance scattering process. This means that it is quite natural for intuitive physical reasons that (3.18) holds only for $t > 0$ and (3.18′) holds only for $t < 0$.

Equation (3.1) gives the probability amplitude for finding the state $\psi^-(t)$, which will be observed in the distant future, $t \to +\infty$, after the interaction has ceased to be effective, as ψ^{out}, if the state of the system is $\phi^+(t)$, which was prepared in the remote past, $t \to -\infty$, before the interaction became effective as ϕ^{in}. If this (for simplicity, two-body) scattering process happens with time delay, i.e., resonance formation, then it is depicted by Fig. 2(a) and (3.1) describes the scattering from an in-state through resonance formation and subsequent decay into an out-state. It leads to the same value at any time $-\infty < t < +\infty$.

In contrast to this whole scattering process, let us now consider a decay process. The decay process is only the "later" half of a resonance scattering process, for which one ignores the formation process; i.e., one does not wish to describe how the resonance developed from ϕ^{in} at $t \to -\infty$ but pays attention only to that part of the full scattering process in which the resonance starts decaying at a given time, say $t = 0$. Thus, one starts the description not with the state ϕ^{in} but with the state $\phi^+(t = 0)$ and such a process would, therefore, be depicted by Fig. 2(b) instead of Fig. 2(a). In such a process one observes the decay product $\psi^{\text{out}}(t)$ only after the time $t = 0$.

Let us now see how this is related to the mathematical conditions (3.12) or (3.13), which was required for the connecting of the pole below the real axis with the decaying Gamow vector (3.15). From the Paley–Wiener theorem [47] follows that (3.13) is fulfilled if and only if

$$\int_{-\infty_{II}}^{-\infty_{II}} dE\, e^{-iEt} \langle {}^-E + i\epsilon | \psi^- \rangle = 0 \quad \text{for } t < 0. \quad (3.22)$$

With (3.3) and (3.2) one obtains[40]

$$\int dE \langle {}^-E | e^{-iHt} | \psi^- \rangle = \int dE \langle E | \psi^{\text{out}}(t) \rangle = 0$$

$$\text{for } t < 0. \quad (3.23)$$

This mean that the integral over the probability amplitude of the decay product for all energies vanishes at times $t < 0$, which may be taken as the mathematical expression for observing the decay product only after $t = 0$. Thus, the mathematical condition for the later half of the resonance scattering process is given by (3.12) or (3.13).

On the other hand, the formation process is the "earlier" half of a resonance scattering process. One ignores the decay process and does not wish to describe how the resonance will develop into ψ^{out} at $t \to \infty$, but describes only that part of the full scattering process in which the resonance has stopped forming at a given time, $t = 0$. In this way one stops

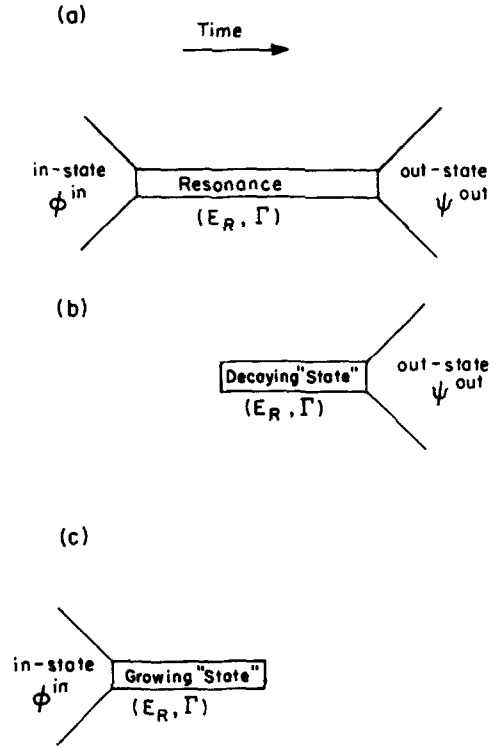

FIG. 2. Separation of resonance scattering (a) into a later (b) and an earlier (c) part. The later part is connected with decay, the earlier part with formation.

the description not with the state ψ^{out} but with the state $\psi^-(t = 0)$, that arose in the transition from $\phi^+(t)$, the state that was prepared as ϕ^{in} at $t \to -\infty$.

This earlier part of the full resonance scattering process will then be depicted by Fig.2(c). In such a process one prepares the state $\phi^{\text{in}}(t)$ only before the time $t = 0$.

Let us now see how this is related to the mathematical condition of (3.12′) or (3.13′), which was required for connecting the pole above the real axis with the growing Gamow vector (3.15′). From the Paley–Wiener theorem[47] follows that (3.13′) is fulfilled if and only if

$$\int_{-\infty_{II}}^{+\infty} dE\, e^{-iEt} \langle {}^+E - i\epsilon | \phi^+ \rangle = 0 \quad \text{for } t > 0. \quad (3.22')$$

With (3.3) and (3.2) one obtains[40]

$$\int dE \langle {}^+E | e^{-iHt} | \phi^+ \rangle = \int dE \langle E | \phi^{\text{in}}(t) \rangle = 0$$

$$\text{for } t > 0. \quad (3.23')$$

This means that the integral over the probability amplitude of the prepared in-state for all energies vanishes at times $t > 0$, which may be taken as the mathematical expression for preparing the intial state only before $t = 0$. Thus, the mathematical condition for the earlier half of the resonance scattering process is given by (3.12′) or (3.13′).

D. New spectral representations for physical states

Equation (2.1) is the well-known energy spectral resolution of a physical state which has been proposed by Dirac and has been proven by the Nuclear Spectral Theorem (if H

also has bound states at E_n then, in addition to the integral, there will be a discrete sum over the E_n). The representations (3.14) and (3.14') are new energy resolutions of physical states. The form (3.14) represents the physical state ϕ^+ as the sum of a decaying "state" with a Breit–Wigner energy distribution plus some background. And the form (3.14') represents the physical state ψ^- as the sum of a growing state with Breit–Wigner energy distribution plus some background. One can rewrite this pair of new generalized eigenvector decomposition (3.14) and (3.14') into a more suggestive form if one eliminates $S(E)$. In order to achieve this, we extend the usual relation

$$|E^+\rangle = |E^-\rangle S(E), \tag{3.24}$$

$$|E^-\rangle = |E^+\rangle S^*(E) \tag{3.24'}$$

to values of E on the negative axis of the second sheet:also

$$|E_{II}^+\rangle = E_{II}^-\rangle S_{II}(E) \quad E < 0 \text{ lower rim} \tag{3.25}$$

and

$$|E_{II}^+\rangle S_{II}(E) = |E_{II}^-\rangle, \quad E < 0 \text{ upper rim} \tag{3.25'}$$

using the symmetry relation of the S matrix,[42] $S^*(E+i\epsilon) = S(E-i\epsilon)$. With this, the normalized Gamow vectors (3.20), (3.20'), (3.20a), and (3.20a') and with

$$s_{-1} = s^*_{-1} = -i\Gamma,$$

one can write (3.14) and (3.14') as

$$\phi^+ = \int_0^{-\infty_{II}} dE\, |E_{II}^+\rangle\langle {}^+E_{II}|\phi^+\rangle + |z_R^-\rangle({}^+z_R|\phi^+) \quad \text{on } \mathscr{H}_+\cap\Phi \tag{3.14a}$$

and

$$\psi^- = \int_0^{-\infty_{II}} dE\, |E_{II}^-\rangle\langle {}^-E_{II}|\psi^-\rangle + |z_R^{*+}\rangle({}^-z_R^*|\psi^-) \quad \text{on } \mathscr{H}\cap\Phi. \tag{3.14a'}$$

These new representations of a physical state look very similar to the Dirac spectral representation, only now the quasistationary states appear in the same place as the bound states in the original spectral representation [it is easily seen that for n pairs of poles one obtains in (3.14a) and (3.14a') a discrete sum over the n Gamow vectors). We will call these representation again spectal representations though the integration and summation runs over values of energy that have nothing to do with the spectrum of H in the Hilbert space sense. These different spectral resolutions provide different realizations of the RHS by spaces of functions.

According to the RHS formulation of quantum mechanics the physically preparable state should be an element of Φ, therefore the Gamow vectors (3.15) and (3.15') cannot represent physically preparable states. A physically preparable decaying state ϕ^+ or growing state ψ^- always contains some background given by the background integral in (3.14) and (3.14'). The decaying "state" vector (Gamow vector)$|z_R^-\rangle$, that originates from the resonance pole of the S matrix below the real axis, is an idealization like the monoenergetic state $|E\rangle$ (Dirac ket), but unlike these it is not even defined as a functional over the whole space of physical states but only over rougly half of all physical states, $\Phi\cap\mathscr{H}_+$. The exponentially growing state vector $|z_R^{*+}\rangle$ that originates from the resonance pole of the S matrix above the real axis is also an idealization and is defined only as a functional over the subspace $\Phi\cap\mathscr{H}_-$. In this way the RHS formulation of quantum mechanics settles the controversy concerning the deviation from the exponential decay law.[5] The resonance *per se* is described by an idealized state vector that develops exponentially in time, but the physically preparable state contains a background term which causes the deviations.

E. Summary of Section 3

We have separated the full resonance scattering process (one pair of poles of the S matrix) into two parts. The growing part (pole in the upper half-plane) is terminated at $t = 0$ by the requirements (3.23') or (3.12'). The state that has arisen through transitions at $t < 0$ from $\phi^+(t)$ is given at $t = 0$ by $|\psi^-\rangle$ of (3.14') and by

$$\psi^-(t) = e^{-iHt}|\psi^-\rangle \quad \text{for } t < 0. \tag{3.26'}$$

Its main contribution is the exponentially growing state $|z_R^{*+}\rangle$, which develops accordings (3.18').

The decaying part (pole in the lower half-plane) is started to be observed at $t = 0$ by the requirment (3.23) or (3.12). The state that decays by transitions at $t > 0$ into $\psi^-(t)$ is given at $t = 0$ by $|\phi^+\rangle$ of (3.14) and by

$$\phi^+(t) = e^{-iHt}|\phi^+\rangle \quad \text{for } t > 0. \tag{3.26}$$

Its main contribution is the exponentially decaying state $|z_R^-\rangle$, which develops according to (3.18).

The space of physical states for the growing part of the scattering process is contained in $\mathscr{H}_-$. For the growing part of the process, $t < 0$, $\psi^-(t)\in\Phi\cap\mathscr{H}_-$ and the growing state $|z_R^{*+}\rangle$ is defined as a functional over $\{\phi^+\}\subset\mathscr{H}_-$. This growing part of the process is described by the primed equations.

The space of physical states for decaying part of the scattering process is contained in $\mathscr{H}_+$. For the decaying part of the process, $t > 0$, $\phi^+(t)\in\Phi\cap\mathscr{H}_+$ and the decaying state $|z_R^-\rangle$ is defined as functional over $\{\psi^-\}\subset\mathscr{H}_-$. This decaying part of the process is described by the unprimed equations. [Note that the same symbols ψ^-, ϕ^+ have different meanings in the growing part (primed equations) and the decaying part (unprimed equations).]

4. SEPARATING THE EXPONENTIALLY DECAYING COMPONENT OF THE DENSITY MATRIX

In this final short section we want to show how the considerations of the preceding section may be related to attempts of the Brussel group[20] to find transformations from the old representation of the density matrix into a new representation in which the exponentially decaying part is separated. This relation can be uncovered if one compares the original generalized basis vector expansion of the vector ϕ^+:

$$\phi^+ = \int_0^\infty dE\,|E^+\rangle\langle{}^+E|\phi^+\rangle$$
$$= \int_0^\infty dE\,|E^-\rangle S(E)\langle{}^+E|\phi^+\rangle \tag{4.1}$$

[integrated along the upper rim, $(E+i\epsilon)$, of the cut in the physical sheet] with the new generalized basis vector expansion (3.14). Equation (3.14a) is a generalized eigenvector expansion of the physical state ϕ^+ in which the idealized decaying state vector ϕ^D is an element of the generalized basis system. It is, therefore, the most suitable choice for an eigenvector expansion of a physical state dominated by a decaying state. The smaller the background term;
$|S_{II}(-E)\langle{}^+ - E_{II}|\phi^+\rangle\Delta E|$ as compared to
$|2\pi i\mathfrak{z}_{-1}\langle{}^+z_R|\phi^+\rangle|$, the closer is ϕ^+ to an idealized (exponentially) decaying state.

We assume now that the values of the analytically continued wavefunctions $\langle\psi^-|E_{II}^+\rangle$ and $\langle{}^+E_{II}|\phi^+|$ fulfill the relation

$$\langle\psi^-|E_{II}{}^+\rangle = -\langle\psi^-|-E_{II}{}^+\rangle,$$
$$\langle{}^+E_{II}|\phi^+\rangle = \langle{}^+-E_{II}|\phi^+\rangle. \tag{4.2}$$

The physical values of the wavefunctions are $\langle E^+|\phi^+\rangle$ for $0 \leqslant E < \infty$ on the physical sheet (upper rim) and whether the analytic continuation can be done such that (4.2) is fulfilled depends upon the particular properties of the space of physical states Φ. This space already has to fulfill many other conditions specified in Sec. 3 and it may well be that (4.2) is in conflict with these conditions.[48] But if one uses (4.2) then (3.14a) becomes

$$\phi^+ = \int_0^\infty dB\,|E_{II}{}^+\rangle\,\langle{}^+E_{II}|\phi^+\rangle + |z_R^-)({}^+z_R|\phi^+). \tag{4.3}$$

From this form one sees, in an obvious way, what is of course also contained in (3.14), namely that the original components (energy wave function) of ϕ^+ have been transformed into new components:

$$\langle E|\phi^{in}\rangle = \langle{}^+E|\phi^+\rangle \to \begin{pmatrix} ({}^+z_R|\phi^+) \\ \langle{}^+E_{II}|\phi^+\rangle \end{pmatrix}, \tag{4.4}$$

in which the exponentially decaying part has been separated. If the wavefunction is transformed by (4.4) then the density matrix of the statistical operator $|\phi^+\rangle\langle\phi^+|$ is transformed according to

$$\langle{}^+E'|\phi^+\rangle\langle\phi^+|E^+\rangle = \rho_{E'E} \to \rho^p_{E'E}$$
$$= \begin{pmatrix} \langle{}^+z_R|\phi^+\rangle\langle\phi^+|z_R^{*+}\rangle & \langle{}^+E'|\phi^+\rangle\langle\phi^+|z_R^*\rangle \\ \langle{}^+z_R|\phi^+\rangle\langle\phi^+|E^+\rangle & \langle{}^+E'|\phi^+\rangle\langle\phi^+|E^+\rangle \end{pmatrix}$$

In more realistic physical situations the state is not described by a projection operator $|\phi^+\rangle\langle\phi^+|$ but by a more general statistical operator (in Φ) W^+. As every W can be given by

$$W^+ = \sum_{i,j} v_{ij}|\phi_i{}^+\rangle\langle\phi_j{}^+| \quad \text{with } \phi_j{}^+, \phi_i{}^+ \in \Phi,$$

the transformation (4.4) has just to be repeated for every i, j in order to accomplish the transformation from the original density matrix $\langle{}^+E'|W^+|E^+\rangle$ into the density matrix in which the exponentially decaying component is separated.

$$\langle{}^+E'|W^+|E^+\rangle \to \begin{pmatrix} \langle{}^+z_R|W^+|z_R^{*+}\rangle & \langle{}^+E|W^+|z_R^*\rangle \\ \langle{}^+z_R|W^+|E^-\rangle & \langle{}^+E'|W^+|E^+\rangle \end{pmatrix}. \tag{4.6}$$

From the following calculations,

$$\langle{}^-z_R|W^+(t)|z_R^{*-+}\rangle = \langle{}^+z_R|e^{iHt}W^+e^{+iHt}|z_R^{*+}\rangle \qquad t \geqslant 0$$
$$= e^{-iz_Rt}e^{iz_R^*t}\langle{}^+z_R|W^+|z_R^{*+}\rangle \tag{4.7}$$
$$= e^{-\Gamma t}\langle{}^+z_R|W^+|z_R^{*+}\rangle,$$

one can see that the exponentially decaying part has been separated, as was demanded in the program of the Brussels group.[20]

ACKNOWLEDGMENTS

This paper was started while visiting the Solvay Institute, and the author would like to express his gratitude to I. Prigonine for the hospitality extended at him at Brussels. He would like to thank him and his colleagues, in particular A. Grecos, C. George, M. de Haan, and F. Mayne, for many valueable discussions which led to the presentation in Sec. 4. For discussion of the mathematical problems that arise in this work, he would like to express his gratitude to I. M. Gelfand, J. E. Gilbert, S. G. Guindikin, A. A. Kirillov, K. Napiorkowski, and M. Gadella. Problems of Sec. 2(b), in particular the nonderivability of the Hilbert space, were discussed with G. Ludwig, O. Melsheimer, and H. Neumann, and the author is grateful for their opinions concerning this point, which were included in Ref. 27. Part of this work was done while at Würzburg University and the author would like to express his gratitude to K. Kraus, who has read several versions and made many suggestions. The author would also like to express his gratitude to M. K. Polivanov and his group at the Steklov Institute and, in particular, to L. A. Khalfin for his suggestions for the final version of this paper. Support from the USDOE (contract No.ERO-3992) and the Alexander von Humboldt Foundation is gratefully acknowledged.

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[22]To complete a space means to adjoin to it the limit elements of Cauchy sequences in a similar manner as one completes the set of rational numbers to obtain the set of real numbers. Topology here is given by specifying the meaning of convergence of infinite sequences (however the topology of $\Phi^\times$ cannot be defined in this way).

[23]Earlier (see Ref. 32 below) it had been suggested that the topology of Φ be defined by the countable number of scalar products $(\phi,\psi)_n = (\phi,(\Delta + 1)^n\psi)$, $n = 0,1,2,3,...$, where $\Delta = \Sigma X_i^2$ is essentially self-adjoint and X_i are the essentially self-adjoint generators of the associative algebra of observables $\mathcal{A}$. If $\mathcal{A}$ is an enveloping algebra of a semisimple group (spectrum-generating, dynamical, or symmetry group) then Φ can be proven to be nuclear [Appendix B of A. Bohm, J. Math. Phys. **8**, 1551 (1967)]. However, a Φ defined by this topology may be already too large for our present purpose.

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[27]It has often been said that the Hilbert space formulation of quantum mechanics can be derived from more physically motivated axioms (Refs. 28–30) Since the topology determines the convergence of infinite sequences, whereas one can only perform a finite number of experiments, this is an entirely unacceptable statement. It is also a misrepresentation of the work in Ref. 28 and 29. How to topologize the set of observables or the set of states cannot be determined from physical arguments alone but should be chosen for mathematical convenience. Only if one chooses for the complete set of states K (see p. 203 of Ref. 29) the *norm-closed* convex set generated by the set of physical states $\mathcal{K}$ (see p. 200 of Ref. 29), does one obtain the Hilbert space $\mathcal{H}$. But instead of choosing the norm-closed K, one may as well choose any subset of K which is obtained from $\mathcal{K}$ by completion with respect to a stronger topology. This one can do in such a way that one is led for the space of (pure) physical states to a subspace Φ of $\mathcal{H}$.

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[36]Section XIV.5 of Ref. 3.

[37]E. g., Sec. XVII. 5 of Ref. 3, or K. Gottfried, *Quantum Mechanics* (Benjamin, New York, 1966), Sec. 14.4.

[38]Chapter IV of Ref. 3. These well-known facts of scattering theory are in every good book on scattering theory, of which R. G. Newton, *Scattering Theory of Waves and Particles* (McGraw-Hill, New York, 1966), is particularly recommendable for the things needed here.

[39]These assumptions are not crucial, as one will see when one goes through the arguments below. If there are N pairs of poles (complex poles of the S matrix always come in pairs), one will obtain N instead of one Gamow vectors. If there are complex cuts, one obtains a different background term, but our arguments concerning the Gamow vectors are unaffected. However, then one will not obtain the representation of Ref. 20. The assumptions (4) and (5) are also not very restrictive: If the S matrix comes form a potential, then for Yukawa-type potentials and for cutoff potentials these conditions will be fulfiled.

[40]The physically accessible quantities are the wavefunctions $|\langle E|\phi^{\text{in}}\rangle| = |\langle {}^+E_{\text{II}} - i\epsilon|\phi^+\rangle| = |\langle {}^+E_{\text{I}} + i\epsilon|\phi^+\rangle|$, $|\langle E|\psi^{\text{out}}\rangle| = |\langle {}^-E_{\text{I}} - i\epsilon|\psi^-\rangle| = |\langle {}^-E_{\text{II}} + i\epsilon|\psi^-\rangle|$ for $0 \leqslant E < \infty$ only. They have to be suitably continued if one needs their values for negative or complex energies. Into which domain of the energy plane they can be continued, and which value they take there, depends upon the properties of the space of physical states Φ which in turn depends, like the S matrix $S(\omega)$, upon the property of the physical system under consideration. It is unlikely that a Φ fulfilling (6) does not exist, but the investigation of the mathematical properties of such Φ's and their reflection upon the physical states remains the principal problem to be solved.

[41]If there are poles and/or cuts along the negative real axis of the second sheet (e.g., in case of Yukawa-type potentials) then the integrals in (3.9) and (3.10) have to be taken along the lower rim of the negative real axis and the integrals in (3.9) and (3.10′) have to be taken along the upper rim of the negative real axis.

[42]E. g., H. M. Nusssenzveig, *Causality and Dispersion Relations* (Academic, New York, 1972), Eqs. (2.8.15).

[43]$G(E) \in L^p_+(E)$ [$\tilde{\mathfrak{H}}^p$-function or H^p-class functions; for $p = 2$ they are called of the Hardy class] iff it is the limit $\eta \to 0$ of a function $G(\omega)$, $\omega = E + i\eta$, that is analytic in the half-plane $\eta \gtrless 0$, such that $|G(E + i\eta)|^p$ is integrable for each $\eta \gtrless 0$ and for which $(\int |G(E + i\eta)|^p dE)^{1/p}$ is bounded for $0 < \eta < \infty$ and $0 > \eta > -\infty$, respectively. For $p = 2, L^2_+(E)$ is the space of Hardy class functions and the space of square integrable functions on the real line $L^2(E)$ is the direct sum $L^2(E) = L^2_+(E) \oplus L^2_-(E)$.

[44]P. L. Duren, *Theory of H^p-Spaces* (Academic, New York, 1970), Theorem 11.8.

[45]E. g., Ref. 3, p. 492.

[46]Note that according to Sec. 2 Eq. (2.6′) our simplified notation $H|z_R^-\rangle = z_R|z_R^-\rangle$ and $e^{-iHt}|z_R^-\rangle = e^{-iz_R t}|z_R^-\rangle$ actually means $\langle\tilde{\psi}|H^\times|z_R^-\rangle = z_R\langle\tilde{\psi}|z_R^-\rangle, \langle\tilde{\psi}|e^{iH^\times t}|z_R^-\rangle = e^{-iz_R t}\langle\tilde{\psi}|z_R^-\rangle$ for every $\tilde{\psi} \in {}_+\cap\Phi$.

[47]E. g., Ref. 44, Theorem 11.9.

[48]This question is under investigation: M. Gadella (to appear).

Perturbed Hamiltonian systems [a)]

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(Received 9 June 1981; accepted for publication 11 August 1981)

It is shown that when a completely integrable Hamiltonian system is perturbed about a particular solution the resulting equations to all orders are completely integrable Hamiltonian systems. Numerous examples are worked out and some new constants for the original system are obtained.

PACS numbers: 03.20. + i, 02.30.Hq

I. INTRODUCTION

In recent years there has been considerable interest in nonlinear evolution equations which can be written in Hamiltonian form. Physically, they are interesting in that they describe relevant phenomena. Mathematically, the interest is in the fact that many of these systems are completely integrable.

Given a particular solution of such an equation (for example, a soliton), it is natural to ask for the behavior of nearby solutions. For example, one might be interested in the stability of the given solution. Here we present a theorem which essentially says that if the original system is completely integrable, then to any order in perturbation theory the resulting equations form a completely integrable Hamiltonian system. Explicit prescriptions for the Hamiltonians, Poisson brackets, and the constants of motion are given. The theorem applies to almost all known completely integrable nonlinear evolution equations. In Sec. IV, we give numerous examples.

II. BASIC THEOREM

Suppose that a nonlinear evolution equation

$$u_t = K(u) \tag{1}$$

can be written in Hamiltonian form, $u_t = [u,\mathscr{H}]$, where the Poisson bracket is antisymmetric and satisfies the Jacobi identity. We look for a solution close to a given solution $u^{(0)}$ of Eq. (1) in the form

$$u = u^{(0)} + \Delta u \tag{2}$$

where $\Delta u = \Sigma_{r=1}^{n} \epsilon^r u^{(r)}$.

(1) Then the equations for $u^{(n)}$ (assuming $u^{(i)}$ $0 \leqslant i < n$ known) form a Hamiltonian system. The Poisson bracket has the same form as the original one, but with $u(x)$ replaced by $u^{(n)}_{(x)}$. The nth Hamiltonian is the coefficient of ϵ^{2n} in the expansion of $\mathscr{H}[u]$.

(2) If the original system is completely integrable, then the equations for $u^{(n)}$ are completely integrable. Indeed, if I_m is a constant for Eq. (1), then the coefficient of ϵ^n in the expansion of I_m is a constant for the equations for $u^{(n)}$.

Proof: We prove these results for a dynamical system specified by a Hamiltonian which is a functional of a single function $u(x,t)$. The generalization to a functional of an arbitrary number of field variables will be obvious. There is no restriction on the dimension of the domain of the field although we consider one space dimension for notational simplicity.

Thus, we have a Hamiltonian $\mathscr{H}[u]$, and the equation of motion is

$$u_t = [u,\mathscr{H}] \tag{3}$$

with the Lie bracket defined by

$$[F_i,F_j] = \int_{-\infty}^{\infty} dy \frac{\delta F_1}{\delta u(y)} \mathscr{O}(\partial_y) \frac{\delta F_2}{\delta u(y)}; \tag{4}$$

$\mathscr{O}(\partial_y)$ is an symplectic, possibly integrodifferential operator which is not field dependent. We wish to determine a bracket $[\ ,\ ]_n$ and a Hamiltonian $\mathscr{H}_n$ such that in substituting (2) into Eq. (3) we can write to each order in ϵ

$$u_t^{(n)} = [u^{(n)},\mathscr{H}_n]_n. \tag{5}$$

The following notation for a functional Taylor expansion is introduced.

$$H[u^{(0)} + \Delta u] = \sum_{N=0}^{\infty} I^N\left(\frac{[\Delta u]^N}{N!} \frac{\delta^n H[u^{(0)}]}{\delta_u N}\right), \tag{6}$$

where

$$I^1\left(\Delta u \frac{\delta H}{\delta u}\right) \equiv \int_{-\infty}^{\infty} dx_1\, \Delta u(x_1) \frac{\delta H}{\delta u(x_1)},$$

$$I^2\left([\Delta u]^2 \frac{\delta^2 H}{\delta u^2}\right) \equiv \int_{-\infty}^{\infty} dx_1 \int_{-\infty}^{\infty} dx_2\, \Delta u(x_1)\Delta u(x_2) \times \frac{\delta^2 H}{\delta u(x_1)\delta u(x_2)}, \quad \text{etc.}$$

On substituting (2) into (6), we find that the coefficient of ϵ^n in the expansion of some functional $H[u]$ is

$$H^{(n)} = \sum_{m_i=0}^{n} \sum_{N=1}^{n} I^N\left(\frac{[u^{(1)}]^{m_1}[u^{(2)}]^{m_2}\cdots[u^{(N)}]^{m_N}}{m_1!m_2!\cdots m_N!} \frac{\delta^N H[u^{(0)}]}{\delta u^N}\right),$$

$$N = m_1 + m_2 + \cdots + m_N,$$

$$n = m_1 + 2(m_2) + \cdots + n(m_n). \tag{7}$$

Define the nth bracket by

$$[F_i,F_j]_n = \int_{-\infty}^{\infty} dy \frac{\delta F_i}{\delta u_{(y)}^{(n)}} \mathscr{O}(\partial_y) \frac{\delta F_j}{\delta u_{(y)}^{(n)}}, \tag{8}$$

and let H_n be $H^{(2n)}$, the coefficient of ϵ^{2n} in the expansion of H. Then, we have Eq. (5) if we can show that

$$(\delta H/\delta u)^{(n)} = \delta H^{(2n)}/\delta u^{(n)}. \tag{9}$$

To prove (9), consider $H^{(2n)}$ as a function of $u^{(n)}$. There are two cases: $m_n = 1, m_n = 2$.

[a)]This work was supported in part by the National Science Foundation under Grand MCS80-17781.

 0022-2488/81/122824-07$01.00

(A) When $m_n = 2$, all the other m_i's are zero and $N = 2$.

$$H^{(2n)} = I^2\left(\frac{[u^{(n)}]^2}{2}\frac{\delta^2 H}{\delta u^2 2}\right) = \int_{-\infty}^{+\infty} dx_1 \int_{-\infty}^{+\infty} dx_2\, u^{(n)}(x_1)u^{(n)}(x_2)\frac{\delta^2 H[u^{(0)}]}{\delta u(x_1)\delta u(x_2)}. \tag{10}$$

Thus,

$$\frac{\delta H^{(2n)}}{\delta u^{(n)}(x)} = \int_{-\infty}^{\infty} dx_1\, u^{(n)}(x_1)\frac{\delta^2 H[u^{(0)}]}{\delta u(x_1)\delta u(x)}. \tag{11}$$

In the particular case that $(\delta H/\delta u)^n$ is an explicit function of $u^{(n)}(x)$, it is equal to (11).

(B) When $m_n = 1$,

$$H^{(2n)} = \sum_{m_i=0}^{n}\sum_{N=2}^{1+n} I^N\left(u^{(n)}\frac{[u^{(1)}]^{m_1}\cdots[u^{(n-1)}]^{m_{n-1}}}{m_1!\cdots m_{n-1}!}\frac{\delta^N H[u^{(0)}]}{\delta u^N}\right),\quad n = m_1 + 2m_2 + \cdots + (n-1)m_{n-1},$$

$$N = 1 + m_1 + \cdots + m_{n-1}$$

$$= \sum_{m_i=0}^{n}\sum_{N=2}^{1+n} I^{N-1}\left(\int_{-\infty}^{\infty} dx_1\, u^{(n)}(x_1)\frac{[u^{(1)}]^{m_1}\cdots[u^{(n-1)}]^{m_{n-1}}}{m_1!\cdots m_{n-1}!}\frac{\delta^N H[u^{(0)}]}{\delta u^{N-1}\delta u(x_1)}\right),\quad n = m_1 + \cdots + (n-1)m_{n-1},$$

$$N = 1 + m_1 + \cdots + m_{n-1}. \tag{12}$$

Thus,

$$\frac{\delta H^{(2n)}}{\delta u^{(n)}(x)} = \sum_{m_i=0}^{n}\sum_{N=2}^{1+n} I^{N-1}\left(\int_{-\infty}^{\infty} dx_1\,\delta(x_1 - x)\frac{[u^{(1)}]^{n_1}\cdots[u^{(n-1)}]^{m_{n-1}}}{m_1!\cdots m_{n-1}!}\frac{\delta^N H[u^{(0)}]}{\delta u^{N-1}\delta u(x_1)}\right),\quad n = m_1 + \cdots + (n-1)m_{n-1},$$

$$N = 1 + m_1 + \cdots + m_{n-1},$$

$$= \sum_{m_i=0}^{n}\sum_{N=1}^{n} I^N\left(\frac{[u^{(1)}]^{n_1}\cdots[u^{(n-1)}]^{m_{n-1}}}{m_1!\cdots m_{n-1}!}\frac{\delta^{N+1}H[u^{(0)}]}{\delta u^N\delta u(x)}\right),\quad n = m_1 + \cdots + (n-1)m_{n-1},$$

$$N = m_1 + \cdots + m_{n-1}. \tag{13}$$

Notice that this expression is $(\delta H/\delta u(x))^{(n)}$ in all cases that that's not a functional of $u^{(n)}$. We have shown (9).

One can readily see that these results also apply when the Hamiltonian system is given in terms of canonical variables (discrete or continuous). For example, in discrete canonical coordinates, the nth Poisson bracket is

$$[F_i, F_j]_n \equiv \sum_{n=1}^{k}\left(\frac{\partial F_i}{\partial q_n^{(n)}}\frac{\partial F_j}{\partial p_n^{(n)}} - \frac{\partial F_j}{\partial q_n^{(n)}}\frac{\partial F_i}{\partial p_n^{(n)}}\right). \tag{14}$$

The nth Hamiltonian is given by the following expression.

$$H_n = \sum_{m_i^j, l_j^i = 0}^{2n}\sum_{N=1}^{2n}\left\{\frac{[q_1^{(1)}]^{m_1^1}\cdots[q_1^{(2n)}]^{m_{2n}^1}\cdots[q_k^{(1)}]^{m_2^k}\cdots[q_k^{(2n)}]^{m_{2n}^k}[p_1^{(1)}]^{l_1^1}\cdots[p_k^{(2n)}]^{l_{2n}^k}}{m_1^1!\cdots m_{2n}^1!\cdots m_1^k!\cdots m_{2n}^k! l_1^1!\cdots l_{2n}^k!}\right\}\cdot\frac{\partial^N H}{\partial q_1^{\alpha^1}\cdots\partial q_k^{\alpha^k}\partial p_1^{\beta^1}\cdots\partial p_k^{\beta^k}},$$

$$2n = m_1^1 + 2m_2^1 + \cdots + 2nm_{2n}^1 + m_1^2 + \cdots + 2nl_{2n}^k,\ \alpha^i = m_1^i + m_2^i + \cdots + m_{2n}^i,$$

$$\beta^i = l_1^i + l_2^i + \cdots + l_{2n}^i, N = \alpha^1 + \cdots + \alpha^k + \beta^1 + \cdots \beta^k. \tag{15}$$

While the perturbation equations are all linear, the existence of the constants is not immediately obvious. In most of the cases we have in mind the equations are inhomogeneous partial differential equations with coefficients which are time and space dependent. Among other things, the H_n are time dependent.

III. THE FIRST-ORDER EQUATIONS

These are clearly the most important and so deserve some special remarks.

(A) As observed elsewhere,[1] the generating function for the conserved densities for many completely integrable nonlinear evolution equations (such as Korteweg–de Vries) obey the first-order perturbation equations. Thus, this generating function itself is the solution of a completely integrable Hamiltonian system. Further, since this function is usually a quadratic function of the eigenfunctions which occur in the inverse scattering method of solution, we obtain from our first-order constants new constants for our original system.

(B) In a sense the above theorem is complementary to a previous theorem.[2] It was shown that if I_m is a constant of our nonlinear system then

$$q^1 = [q^{(0)}, I_m], \quad p^{(1)} = [p^{(0)}, I_m] \tag{16}$$

is a solution of the first-order equations. For such solution (since they are known explicitly), we have no need of constants of motion. However, it is interesting to see what the constants are for such solutions.

Theorem: If

$$[I_n, I_m] = 0, \tag{17}$$

i.e., the two constants are in involution, then

$$I_m^{(1)}(q^{(1)},p^{(1)}) = 0. \tag{18}$$

Proof:

$$I_m^{(1)} = \sum_l \frac{\partial I_m}{\partial q_l^{(0)}} q_l^{(1)} + \frac{\partial I_m}{\partial p_l^{(0)}} p_l^{(1)}, \tag{19}$$

but from Eq. (16)

$$q_l^{(1)} = \frac{\partial I_n}{\partial p_l^{(0)}}, \quad p_l^{(1)} = \frac{-\partial I_n}{\partial q_l^{(0)}} \tag{20}$$

$$\therefore I_m^{(1)} = \sum_l \left\{ \frac{\partial I_m}{\partial q_l^{(0)}} \frac{\partial I_n}{\partial p_l^{(0)}} - \frac{\partial I_m}{\partial p_l^{(0)}} \frac{\partial I_n}{\partial q_l^{(0)}} \right\} = [I_m, I_n] = 0. \tag{21}$$

In particular the two obvious solutions of the equations obtained by linearizing around a solution $u^{(0)}$ of an originally not explicitly time and space dependent evolution equation, $u_t^{(0)}$ and $u_x^{(0)}$ are such that the constants $I_m^{(1)}$ for these solutions are all zero. [The solutions are generated from Eq. (16) using the energy and momentum.]

IV. EXAMPLES

For the first example we consider the Korteweg–de Vries equation.

A. The KdV equation

Take this in the form

$$u_t = -\partial_x \{u^2 + 2u_{xx}\}. \tag{22}$$

It is

$$u_t = [u, \mathscr{H}], \tag{23}$$

where

$$[F_i, F_j] = \int_{-\infty}^{\infty} \frac{\delta F_i}{\delta u} (-\partial_x) \frac{\delta F_j}{\delta u} dx \tag{24}$$

and

$$\mathscr{H} = \int_{-\infty}^{\infty} \frac{u^3}{3} - (u_x)^2 dx. \tag{25}$$

As is well known, there are an infinite number of polynomial constants. The first few are

$$I_1 = \int_{-\infty}^{\infty} u\, dx, \quad I_2 = \int_{-\infty}^{\infty} \frac{u^2}{2} dx, \quad I_3 \equiv \mathscr{H},$$

$$I_4 = \int_{-\infty}^{\infty} \left\{ 2u_{xx}^2 - \tfrac{10}{3} u (u_x)^2 + \tfrac{5}{18} u^4 \right\} dx.$$

$$H_2 = H^{(4)} = \int_{-\infty}^{\infty} dx\, u^{(4)} \frac{\delta H}{\delta u(x)} + \int_{-\infty}^{\infty} dx\, dy \left(u^{(1)}(x) u^{(3)}(y) + \frac{u^{(2)}(x) u^{(2)}(y)}{2!} \right) \frac{\delta^2 H}{\delta u(x) \delta u(y)} + \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} du \int_{-\infty}^{\infty} dz \frac{u^{(1)}(x) u^{(1)}(y) u^{(2)}(z)}{2!} \frac{\delta^3 H}{\delta u(x) \delta u(y) \delta u(z)}$$

$$= \int_{-\infty}^{\infty} dx \left(u^{(4)} \{[u^{(0)}]^2 + 2u_{xx}^{(0)}\} + u^{(3)} \{2u^{(1)} u^{(0)} + 2u_{xx}^{(0)}\} + [u^{(2)}]^2 u^{(0)} - [u_x^{(2)}]^2 + [u^{(1)}(x)]^2 u^{(2)}(x) \right). \tag{34}$$

The equation of motion is

$$u_t^{(2)} = -\partial_x \{2u^{(0)} u^{(2)} + (u^{(1)})^2 + 2u_{xx}^{(2)}\}. \tag{35}$$

First-order equations: Write

$$u = u^{(0)} + \epsilon u^{(1)} + \epsilon^2 u^{(2)}. \tag{26}$$

Inserting in $\mathscr{H}$ and identifying ϵ^2 terms yields

$$\mathscr{H}_1 = \int_{-\infty}^{\infty} \{u^{(0)}(u^{(1)})^2 - (u_x^{(1)})^2 + [(u^{(0)})^2 + u_{xx}^{(0)}] u^{(2)}\} dx. \tag{27}$$

Now with $[F_i, F_j] = \int_{-\infty}^{\infty} \delta F_i/\delta u^{(1)} (-\partial_x) \delta F_j/\delta u^{(1)}\, dx$ we obtain the (correct) linearized equation

$$u_t^{(1)} = [u^{(1)}, \mathscr{H}_1]_1 = -\partial_x \{2u^{(0)} u^{(1)} + 2u_{xx}^{(1)}\}. \tag{28}$$

First-order constants: Insert Eq. (26) in I_n and find the coefficient of ϵ. We obtain as constants [for Eq. (28)]

$$I_n^{(1)} = \int_{-\infty}^{\infty} \frac{\delta I_n}{\delta u} u^{(1)} dx. \tag{29}$$

Thus,

$$I_1^{(1)} = \int_{-\infty}^{\infty} u^{(1)} dx, \quad I_2^{(1)} = \int_{-\infty}^{\infty} u^{(0)} u^{(1)} dx, \tag{30}$$

$$I_3 = \int_{-\infty}^{\infty} \{[u^{(0)}]^2 + 2u_{xx}^{(0)}\} u^{(1)} dx \tag{31}$$

$$I_4^{(1)} = \int_{-\infty}^{\infty} \left| 4u_{xxxx}^{(0)} + \tfrac{20}{3} u^{(0)} u_{xx}^{(0)} + \tfrac{10}{3} (u_x^{(0)})^2 + \tfrac{10}{9} [u^{(0)}]^3 \right| \times u^{(1)} dx. \tag{32}$$

Now if ψ is the function in the scattering problem for the inverse scattering method, i.e.,

$$(\partial_x^2 + u/6)\psi = (\lambda/4)\psi, \tag{33}$$

then we know[1] $\Psi = \partial_x \psi^2$ satisfies Eq. (28). The Eqs. (29)–(32) become the constants

$$I_1^{(1)} = 0, \quad I_2^{(1)} = \int_{-\infty}^{\infty} -u_x^{(0)} \psi^2 dx,$$

$$I_3^{(1)} = \int_{-\infty}^{\infty} -\partial_x [(u^{(0)})^2 + 2u_{xx}^{(0)}] \psi^2 dx,$$

$$I_4^{(1)} = \int_{-\infty}^{\infty} -\partial_x \left| 4u_{xxxx}^{(0)} + \tfrac{20}{3} u^{(0)} u_{xx}^{(0)} + \tfrac{10}{3} (u_x^{(0)})^2 + \tfrac{10}{9} (u^{(0)})^3 \right| \psi^2 dx.$$

Second-order equations:

Second-order constants:

$$I_n^{(2)}[u] = \int_{-\infty}^{\infty} dx\, u^{(2)} \frac{\delta I_n[u^{(0)}]}{\delta u(x)} + \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dy \frac{u^{(1)}(x)u^{(1)}(y)}{2!} \frac{\delta^2 I_n[u^{(0)}]}{\delta u(x)\delta u(y)}. \quad (36)$$

Thus,

$$I_1^{(2)} = \int_{-\infty}^{\infty} u^{(2)} dx,\ I_2^{(2)} = \int_{-\infty}^{\infty} \left(u^{(0)}u^{(2)} + \frac{[u^1]^2}{2} \right) dx \quad (37)$$

$$I_3^{(2)} = \int_{-\infty}^{\infty} \{[u^{(0)}]^2 + 2u_{xx}^{(0)}\}u^{(2)} + u^{(0)}[u^{(1)}]^2 - [u_x^{(1)}]^2\, dx \quad (38)$$

$$I_4^{(2)} = \int_{-\infty}^{\infty} \{ [\, u_{xxxx}^{(0)} + \tfrac{10}{3}[u_x^{(0)}]^2 + \tfrac{20}{3}u^{(0)}u_{xx}^{(0)} + \tfrac{10}{9}[u^{(0)}]^3 \,] u^{(2)} + 2[u_{xx}^{(1)}]^2 + \tfrac{5}{3}[u^{(0)}]^2[u^{(1)}]^2 + \tfrac{10}{3}u^{(0)}([u_x^{(1)}]^2 + 2u^{(1)}u_{xx})\} \, dx. \quad (39)$$

B. The KdV hierarchy

It is well known that the polynomial constants for the KdV equation are all in involution. Accordingly, any of them can be used as a Hamiltonian and the constants are all constants of the new equation of motion. In the formulation of Ref. 1 this can be put so:

Let $\mathscr{L}$ be the operator such that

$$\mathscr{L}(\phi) = \partial_x^2\phi + \tfrac{2}{3}u\phi - \tfrac{1}{3}\partial_x^{-1}(u_x\phi). \quad (40)$$

The general equation associated with the hierarchy of KdV equations can be written

$$u_t = -\partial_x f(\mathscr{L})u, \quad (41)$$

where f is an arbitrary entire function. (The connection with the formulation in Ref. 3 is given in Appendix A.)

In particular if we take $f(\mathscr{L}) = \mathscr{L}^2$, we get the equation with I_4 as Hamiltonian. The equation of motion is (using the same Poisson bracket)

$$u_t = -\partial_x \{ 4u_{xxxx} + \tfrac{10}{9}u^3 + \tfrac{10}{3}(u_x)^2 + \tfrac{20}{3}uu_{xx} \}. \quad (42)$$

First-order equations: Giving only those terms which involve $u^{(1)}$, we have

$$\mathscr{H}_1 = \int_{-\infty}^{\infty} \{ 2(u_{xx}^{(1)})^2 - \tfrac{10}{3}u_x^{(0)}(u_x^{(1)})^2 - \tfrac{20}{3}u_x^{(0)}u^{(1)}u_x^{(1)} + \tfrac{5}{3}(u^{(0)})^2(u^{(1)})^2 \}\, dx \quad (43)$$

from the which the first-order equation is

$$u_t^{(1)} = -\partial_x \{ 4u_{xxxx}^{(1)} + \tfrac{10}{3}(u^{(0)})^2u^{(1)} + \tfrac{20}{3}u_x^{(0)}u_x^{(1)} + \tfrac{20}{3}u^{(0)}u_{xx}^{(1)} + \tfrac{20}{3}u^{(1)}u_{xx}^{(0)} \}. \quad (44)$$

The first-order constants are, of course, exactly those for the KdV equations.

C. The Toda lattice

This is of interest in that we use explicitly canonical coordinates and momenta. The connection with the classical literature[4] becomes apparent.

Here

$$\mathscr{H} = \sum_m \left\{ e^{-(q_m - q_{m-1})} - 1 + \frac{p_m^2}{2} \right\} \quad (45)$$

with the equations of motion

$$\dot{q}_i = p_i,\quad \dot{p}_i = -\{ e^{-(q_{i+1} - q_i)} - e^{-(q_i - q_{i-1})} \}. \quad (46)$$

The first three constants are

$$I_1 = \sum_m p_m,\quad I_2 = \mathscr{H},$$

$$I_3 = \sum_m \left\{ [e^{-(q_m - q_{m-1})} - 1][p_{m-1} + p_m] + \frac{p_m^3}{3} \right\}.$$

The first-order Hamiltonian is

$$\mathscr{H}_1 = \sum_m \left\{ e^{-(q_m^{(0)} - q_{m-1}^{(0)})} \frac{(q_m^{(1)} - q_{m-1}^{(1)})^2}{2} + \frac{(p_m^{(1)})^2}{2} \right\}. \quad (47)$$

The equations

$$\dot{q}_i^{(1)} = \partial\mathscr{H}^{(1)}/\partial p_i^{(1)},\quad \dot{p}_i = -\partial\mathscr{H}/\partial q_i^{(1)} \quad (48)$$

are indeed

$$\dot{q}_i^{(1)} = \dot{p}_i^{(1)},$$

$$\dot{p}_i^{(1)} = \{ e^{-(q_{i+1}^{(0)} - q_i^{(0)})}(q_{i+1}^{(1)} - q_i^{(1)}) - e^{-(q_i^{(0)} - q_{i-1}^{(0)})}(q_i^{(1)} - q_{i-1}^{(1)}) \}. \quad (49)$$

The constants for Eqs. (49) are the first-order integral invariants[4]:

$$I_n^{(1)} = \sum_l \left\{ \frac{\partial I_n}{\partial q^{(0)}} q_l^{(1)} + \frac{\partial I_n}{\partial p^{(0)}} p_l^{(1)} \right\}. \quad (50)$$

The simplest of these are

$$I_i^{(1)} = \sum_m p_m^{(1)}, \quad (51)$$

$$I_2^{(1)} = -\sum_m e^{-(q_m^{(0)} - q_{m-1}^{(0)})}(q_m^{(1)} - q_{m-1}^{(1)}) + \sum_m p_m^{(0)}p_m^{(1)}, \quad (52)$$

and

$$I_3^{(1)} = \sum_m (p_m^{(0)})^2 p_m^{(1)} - (p_m^{(1)} + p_{m-1}^{(1)}) + e^{-(q_m^{(0)} - q_{m-1}^{(0)})} \times \{ (p_{m-1}^{(1)} + p_m^{(1)}) - (q_m^{(1)} - q_{m-1}^{(1)})(p_{m-1}^{(0)} + p_m^{(0)}) \}. \quad (53)$$

The Toda lattice is also a member of a hierarchy and thus we have an analogous set of results when any of the constants I_n are used as Hamiltonian.

D. The Benjamin–Ono equation

This we take in the form

$$u_t = -\partial_x \{ u^2 + H[u_x] \}, \quad (54)$$

where the Hilbert transform H is

$$H[\Phi] = +\frac{P}{\pi} \int_{-\infty}^{\infty} \frac{\Phi(x')}{x' - x} dx'. \quad (55)$$

This system is Hamiltonian with

$$\mathscr{H} = \int_{-\infty}^{\infty} \left(\frac{u^3}{3} + \frac{uH[u_x]}{2} \right) dx \quad (56)$$

and Poisson bracket as given by Eq. (24).

The first four constants are

$$I_1 = \int_{-\infty}^{\infty} u\, dx,\quad I_2 = \int_{-\infty}^{\infty} \frac{u^2}{2} dx,\quad I_3 = \mathscr{H},$$

$$I_4 = \int_{-\infty}^{\infty} \left(\frac{u^4}{4} + \tfrac{3}{4}u^2H[u_x] + \frac{u_x^2}{2} \right) dx.$$

We obtain, on keeping only terms proportional to $u^{(1)}$,

$$\mathscr{H}_1 = \int_{-\infty}^{\infty} \left\{ u^{(0)}(u^{(1)})^2 + \frac{u^{(1)} H u_x^{(1)}}{2} \right\} dx, \tag{57}$$

and then

$$u_t^{(1)} = -\partial_x \{ 2u^{(0)}u^{(1)} + H[u_x^{(1)}] \}. \tag{58}$$

First-order constants (among others) are

$$\begin{aligned} I_1^{(1)} &= \int_{-\infty}^{\infty} u^{(1)}\, dx, \\ I_2^{(1)} &= \int_{-\infty}^{\infty} u^{(0)}u^{(1)}\, dx, \\ I_3^{(1)} &= \int_{-\infty}^{\infty} \{ [u^{(0)}]^2 u^{(1)} + u^{(1)} H[u_x^{(0)}] \}\, dx, \\ I_4^{(1)} &= \int_{-\infty}^{\infty} \{ [u^{(0)}]^3 u^{(1)} + \tfrac{3}{2} u^{(0)}u^{(1)} H[u_x^{(0)}] \\ &\quad + \tfrac{3}{4}[u^{(0)}]^2 H[u_x^{(1)}] + u_x^{(0)} u_x^{(1)} \}\, dx. \end{aligned} \tag{59}$$

In second order, again retaining only those terms involving $u^{(2)}$, we have

$$\mathscr{H}_2^{(2)} = \int_{-\infty}^{\infty} \left\{ u^{(0)}[u^{(2)}]^2 + u^{(2)}[u^{(1)}]^2 + \frac{u^{(2)} H[u_x^{(2)}]}{2} \right\} dx, \tag{60}$$

from which follows

$$u_t^{(2)} = -\partial_x \{ 2u^{(0)}u^{(2)} + [u^{(1)}]^2 + H[u_x^{(2)}] \}. \tag{61}$$

Some second-order constants are

$$\begin{aligned} I_1^{(2)} &= \int_{-\infty}^{\infty} u^{(2)}\, dx, \\ I_2^{(2)} &= \int_{-\infty}^{\infty} \left\{ u^{(0)}u^{(2)} + \frac{[u^{(1)}]^2}{2} \right\} dx, \\ I_3^{(2)} &= \int_{-\infty}^{\infty} \{ [u^{(0)}]^2 u^{(2)} + u^{(0)}[u^{(1)}]^2 + u^{(2)} H[u_x^{(0)}] \}\, dx, \\ I_4^{(2)} &= \int_{-\infty}^{\infty} \{ [u^{(0)}]^3 u^{(2)} + \tfrac{3}{2}[u^{(0)}]^2 [u^{(1)}]^2 \\ &\quad + \tfrac{3}{4}[u^{(0)}]^2 H[u_x^{(2)}] \\ &\quad + \tfrac{3}{2} u^{(0)}u^{(1)} H[u_x^{(1)}] + \tfrac{3}{2} u^{(0)}u^{(2)} H[u_x^{(0)}] \\ &\quad + \tfrac{3}{4}[u^{(1)}]^2 H[u_x^{(0)}] + u_x^{(0)}u_x^{(2)} + [u_x^{(1)}]^2/2 \}\, dx. \end{aligned} \tag{62}$$

Again the BO equation is a member of hierarchy of equations. Any of the constants can be chosen as Hamiltonian. The constants for the perturbation equations are all the same.

V. THE HARRY-DYM EQUATION

We consider this since the Poisson bracket is slightly different. The equation is

$$u_t = (\partial_x)^3 u^{-1/2}. \tag{63}$$

Some constants are

$$\begin{aligned} I_1 &= \int_{-\infty}^{\infty} u\, dx, \quad I_2 = 2\int_{-\infty}^{\infty} u^{1/2}\, dx, \\ I_3 &= \int_{-\infty}^{\infty} \frac{u^{-5/2}(u_x)^2}{8}\, dx. \end{aligned} \tag{64}$$

This is Hamiltonian with $\mathscr{H} = I_2$ and

$$[F_i, F_j] = \int_{-\infty}^{\infty} \frac{\partial F_i}{\delta u} (\partial_x)^3 \frac{\delta F_j}{\delta u}\, dx. \tag{65}$$

The first-order Hamiltonian is

$$\mathscr{H}^{(1)} = -\tfrac{1}{8}\int_{-\infty}^{\infty} [u^{(1)}]^2 [u^{(0)}]^{-3/2}\, dx, \tag{66}$$

giving rise to the equation

$$u_t^{(1)} = -\tfrac{1}{4}\partial_x^3 [[u^{(0)}]^{-3/2} u^{(1)}]. \tag{67}$$

The simplest three first-order constants are

$$I_1^{(1)} = \int_{-\infty}^{\infty} u^{(1)}\, dx, \quad I_2^{(1)} = \int_{-\infty}^{\infty} [u^{(0)}]^{-1/2} u^{(1)}\, dx,$$

and

$$I_3^{(1)} = \int_{-\infty}^{\infty} \left\{ \frac{u_x^{(0)}[u^{(0)}]^{-5/2}}{4} u_x^{(1)} - \tfrac{5}{16}[u^{(0)}]^{-7/2}[u_x^{(0)}]^2 u^{(1)} \right\} dx. \tag{68}$$

In second order we obtain

$$\begin{aligned} \mathscr{H}_2 &= \int_{-\infty}^{\infty} \left\{ -\frac{(u^{(2)})^2}{4} (u^{(0)})^{-3/2} + \tfrac{3}{8}(u^{(1)})^2 (u^{(0)})^{-5/2} u^{(2)} \right\} dx, \\ u_t^{(2)} &= \partial_x^3 \{ -\tfrac{1}{2} u^{(2)} (u^{(0)})^{-3/2} + \tfrac{3}{8}(u^{(1)})^2 (u^{(0)})^{-5/2} \}, \\ I_1^{(2)} &= \int_{-\infty}^{\infty} u^{(2)}\, dx, \\ I_2^{(2)} &= \int_{-\infty}^{\infty} \{ 2u^{(2)}(u^{(0)})^{-1/2} - \tfrac{1}{4}(u^{(1)})^2 (u^{(0)})^{-3/2} \}\, dx, \\ I_3^{(2)} &= \tfrac{1}{8}\int_{-\infty}^{\infty} \{ (u^{(0)})^{-5/2}(u_x^{(1)})^2 - 5[u^{(0)}]^{-7/2} \\ &\quad \times \{ [u_x^{(0)}]^2/2u^{(2)} + u^{(1)}u_x^{(1)}u_x^{(0)} \} \\ &\quad + \tfrac{35}{8}[u^{(0)}]^{-9/2}[u^{(1)}]^2 [u_x^{(0)}]^2 \}\, dx, \end{aligned} \tag{69}$$

where again for the Hamiltonian we gave only those terms involving $u^{(2)}$.

We note that Eq. (63) is a member of a hierarchy. The next simplest member is obtained by taking I_3 as the Hamiltonian.

It may also be mentioned[1] that there is an inverse scattering problem associated with Eq. (63). The eigenvalue problem is $\partial_x^2 \psi = \lambda u/2\psi$. Since $\Psi = \partial_x^3 \psi^2$ satisfies Eq. (67), we conclude that the $I_n^{(1)}$ with $u^{(1)}$ replaced by $\partial_x^3 \psi^2$ gives a new set of constants for Eq. (63).

VI. THE AKNS EQUATIONS

In Ref. (3) is what appears to be a very large class of completely integrable systems. It will be seen in Appendix A that the only equations included there have not been discussed are

(i) The hierarchy of modified KdV equations,

(ii) The hierarchy of nonlinear Schrödinger equations,

(iii) The sine-Gordon and the sinh-Gordon equation in light cone coordinates.

There are really two modified KdV hierarchies—depending on the sign of the nonlinear term. The sine-Gordon equation is associated with one of these[1] and the sinh-Gordon with the other.

A. Modified KdV equation

The equation is taken in the form

$$u_t = -\partial_x^3 u - (\partial_x u)^3/2. \tag{70}$$

This is Hamiltonian with

$$\mathscr{H} = I_2 = \int_{-\infty}^{\infty} \left\{ -\frac{(u_{xx})^2}{2} + \frac{(u_x)^4}{8} \right\} dx \tag{71}$$

and

$$[F_i, F_j] = \int_{-\infty}^{\infty} \frac{\delta F_i}{\delta u} (\partial_x^{-1}) \frac{\delta F_j}{\delta u} dx. \tag{72}$$

Some constants in addition to I_2 are

$$I_1 = \int_{-\infty}^{\infty} \frac{(u_x)^2}{2} dx,$$

$$I_3 = \int_{-\infty}^{\infty} \left\{ \frac{u_{xxx}^2}{2} + \frac{3(u_x)^6}{48} - \tfrac{5}{4} u_{xx}^2 u_x^2 \right\} dx. \tag{73}$$

It has been shown[1] that Eq. (70) has the same constants as the sine-Gordon equation. Therefore, another constant is

$$\bar{I} = \int_{-\infty}^{\infty} [1 - \cos u] \, dx. \tag{74}$$

To first-order we have

$$\mathscr{H}_1 = \int_{-\infty}^{\infty} \left\{ -\frac{(u_{xx}^{(1)})^2}{2} + \tfrac{3}{4} (u_x^{(0)})^2 (u_x^{(1)})^2 \right\} dx \tag{75}$$

and

$$u_t^{(1)} = \{ -u_{xxx}^{(1)} - \tfrac{3}{2} (u_x^{(0)})^2 u_x^{(1)} \}. \tag{76}$$

The constants become

$$I_1^{(1)} = \int_{-\infty}^{\infty} u_x^{(0)} u_x^{(1)} \, dx,$$

$$I_2^{(1)} = \int_{-\infty}^{\infty} \left\{ -u_{xx}^{(0)} u_{xx}^{(1)} + \frac{[u_x^{(0)}]^3 u_x^{(1)}}{2} \right\} dx,$$

$$I^{(1)} = \int_{-\infty}^{\infty} \left\{ (u_{xxx}^{(0)}) u_{xxx}^{(1)} + \frac{(u_x^{(0)})^5}{8} u_x^{(1)} - \tfrac{5}{2} u_{xx}^{(0)} (u_x^{(0)})^2 u_{xx}^{(1)} \right.$$

$$\left. - \tfrac{5}{2} (u_{xx}^{(0)})^2 u_x^{(0)} u_x^{(1)} \right\} dx, \tag{77}$$

and

$$\bar{I}^{(1)} = \int_{-\infty}^{\infty} u^{(1)} \sin u^{(0)} \, dx. \tag{78}$$

B. Sine-Gordon equation

Take in the form

$$u_t = \partial_x^{-1} \sin u, \tag{79}$$

which is Hamiltonian with $\mathscr{H} = \bar{I}$ and P. B. as in Eq. (72). The constants are just as for the modified KdV equation.

The inverse scattering method can be applied to the Eq. (79). The eigenvalue problem can be used in the form

$$v_{1x} + \tfrac{1}{2}(\lambda)^{1/2} v_1 = -\tfrac{1}{2} i u_x v_2,$$

$$v_{2x} - \tfrac{1}{2}(\lambda)^{1/2} v_2 = \tfrac{1}{2} i u_x v_1. \tag{80}$$

Then $\partial_x^{-1} \Psi = \partial_x^{-1} [(v_1)^2 - (v_2)^2]$ is a solution of the linearized form of Eq. (79),

$$u_t^{(1)} = \partial_x^{-1} [u^{(1)} \cos u^{(0)}]. \tag{81}$$

Thus putting Ψ in Eqs. (77) and (78), yields new constants for Eq. (79).

C. Nonlinear Schrödinger equation

We take this in the form

$$u_t = i\{u_{xx} + 2\sigma u^2 \bar{u}\}$$

$$\bar{u}_t = -i\{\bar{u}_{xx} + 2\sigma \bar{u}^2 u\} \qquad ,\sigma = \pm 1. \tag{82}$$

This is Hamiltonian with

$$\mathscr{H} = \int_{-\infty}^{\infty} \{(\partial_x \bar{u})(\partial_x u) - \sigma(u\bar{u})^2\} dx \tag{83}$$

and

$$[F_i, F_j] = i \int_{-\infty}^{\infty} \left\{ \frac{\delta F_i}{\delta \bar{u}} \frac{\delta F_j}{\delta u} - \frac{\delta F_i}{\delta u} \frac{\delta F_j}{\delta \bar{u}} \right\} dx. \tag{84}$$

To first order keeping only terms proportional of $u^{(1)}$, we obtain

$$\mathscr{H}_1 = \int_{-\infty}^{\infty} \{(\partial_x \bar{u}^{(1)})(\partial_x u^{(1)}) - 4\sigma \bar{u}^{(0)} u^{(0)} \bar{u}^{(1)} u^{(1)}$$

$$- \sigma(\bar{u}^{(0)})^2 (u^{(1)})^2 - \sigma(u^{(0)})^2 (\bar{u}^{(2)})^2\} dx. \tag{85}$$

From this the perturbed equations are

$$u_t^{(1)} = i\{\partial_x^2 u^{(1)} + 4\sigma(\bar{u}^{(0)})^2 u^{(1)} + 2\sigma(u^{(0)})^2 \bar{u}^{(1)}\} \tag{86}$$

and the complex conjugate equation. The constants are

$$I_1 = \int_{-\infty}^{\infty} \bar{u} u \, dx, \quad I_2 = \frac{1}{i} \int_{-\infty}^{\infty} (\bar{u} \partial_x u) \, dx,$$

$$I_3 = \int_{-\infty}^{\infty} (\bar{u}_x u_x - \sigma(\bar{u}u)^2) \, dx.$$

First-order constants are then

$$I_1^{(1)} = \int_{-\infty}^{\infty} \{\bar{u}^{(0)} u^{(1)} + u^{(0)} \bar{u}^{(1)}\} \, dx,$$

$$I_2^{(1)} = \frac{1}{i} \int_{-\infty}^{\infty} \{\bar{u}^{(0)} \partial_x u^{(1)} + \bar{u}^{(1)} \partial_x u^{(0)}\} \, dx,$$

$$I_3^{(1)} = \int_{-\infty}^{\infty} \{(\partial_x \bar{u}^{(0)})(\partial_x u^{(1)}) + (\partial_x u^{(0)})(\partial_x \bar{u}^{(1)})$$

$$- 2\sigma(u^{(0)})^2 \bar{u}^{(0)} \bar{u}^{(1)} - 2\sigma(\bar{u}^{(0)})^2 u^{(0)} u^{(1)}\} \, dx. \tag{87}$$

ACKNOWLEDGMENT

K. M. Case would like to thank The Institute for Advanced Study for hospitality during part of the time this work was done.

APPENDIX A: RELATION TO AKNS[3] EQUATIONS

In Ref. 4 two general classes of equations are presented:

(1) Those which have the Schrödinger equation as eigenvalue problem, i.e.,

$$v_{xx} + (\rho^2 + u(x,t)/6)v = 0. \tag{A1}$$

The form given was

$$q_t + \hat{C}(4L^+) q_x = 0, \tag{A2}$$

where

$$L^+ = -\frac{1}{4} \frac{\partial^2}{\partial x^2} - q - \tfrac{1}{2} q_x \partial_x^{-1} \tag{A3}$$

and $\hat{C}$ is an arbitrary entire function.

However, in Ref. 1 it is shown from the existence of a dual Hamiltonian formalism that the equation using the nth polynomial constant as Hamiltonian is

$$u_t = -\partial_x Q_n, \tag{A4}$$

where the conserved densities are connected by an operator $\mathscr{L}$ such that

$$Q_{n+1} = \mathscr{L} Q_n. \tag{A5}$$

Clearly, a general equation constructed from the hierarchy is

$$u_t = -\partial_x f(\mathscr{L})u. \tag{A6}$$

Now what is the connection with Eq. (B2). Note that if L_s^+ is given by Eq. (B3) then

$$4L = -\partial_x^2 - 4q + 2\partial_x^{-1} q_x. \tag{A7}$$

We readily check that

$$4L^+ \partial_x = \partial_x 4L. \tag{A8}$$

Hence Eq. (B2) is

$$q_t = -\partial_x \hat{C}(4L)q \tag{A9}$$

which is just Eq. (B6)

We conclude that

(i) All equations of this class are completely integrable Hamiltonian systems.

(ii) The perturbation equations are, to all orders, complete integrable Hamiltonian systems.

(iii) The constants are just those for the KdV equation.

(2) The second general class given in Ref. 5 are equations associated with the Zakharov–Shabat eigenvalue problem. It is

$$\begin{pmatrix} r_t \\ -q_t \end{pmatrix} + 2A_0(L^+)\begin{pmatrix} r \\ q \end{pmatrix} = 0 \tag{A10}$$

with

$$L^+ = \frac{1}{2i}\begin{pmatrix} \partial_x - 2r\partial_x^{-1} q & 2r\partial_x^{-1} r \\ -2q\partial_x^{-1} q & -\partial_x + 2q\partial_x^{-1} r \end{pmatrix}. \tag{A11}$$

The interesting cases seem to be

$$r = \sigma \bar{q} \tag{A12}$$

or

$$r = \sigma q \tag{A13}$$

where $\sigma = \pm 1$.

Now we maintain that the case Eq. (A12) is just the general equation of the nonlinear Schrödinger hierarchy and the case of Eq. (A13) is the modified KdV hierarchy.

In Ref. 5 it was shown that the equations using the nth polynomial constant for the nonlinear Schrödinger equation as Hamiltonian is

$$u_t = -iQ_n,$$

where

$$Q_{n+1} = \mathscr{L} Q_n$$

and $\mathscr{L}(\phi) = -i\{\phi_x + 2\sigma u \partial_x^{-1}(\bar{u}\phi - u\bar{\phi})\}$. But identifying $r = \sigma\bar{u}$, $q = u$ in Eq. (11) just gives $u_t = -if(\mathscr{L})u$ and the complex conjugate.

The case of Eq. (A13) is more amusing. Since the cases $\sigma = \pm 1$ are so similar, for definiteness we consider $\sigma = +1$.

In Ref. 1 we have ssen that the nth member of the modified KdV hierarchy could be written in Hamiltonian form with

$$[F_i, F_j] = \int_{-\infty}^{\infty} \frac{\delta F_i}{\delta u}(-\partial_x)\frac{\delta F_j}{\delta u}\,dx.$$

The nth equation was

$$u_t = -\partial_x Q_n,$$

where

$$Q_{n+1} = \mathscr{L} Q_n$$

and

$$\mathscr{L} = \partial_x^2 - 4u\partial_x^{-1} u\partial_x.$$

Now consider the term in (A10) corresponding to any power of L in Eq. (10). Since now

$$L_+ \sim \begin{pmatrix} \partial_x - 2u\partial_x^{-1} u & 2u\partial_x^{-1} u \\ -2u\partial_x^{-1} u & -\partial_x + 2u\partial_x^{-1} u \end{pmatrix},$$

we have

$$L_+\begin{pmatrix} v \\ v \end{pmatrix} \sim \begin{pmatrix} \partial_x v \\ -\partial_x v \end{pmatrix}$$

and

$$(L_+)\begin{pmatrix} w \\ -w \end{pmatrix} \sim \begin{pmatrix} \partial_x w - 4u\partial_x^{-1} uw \\ \partial_x w - 4u\partial_x^{-1} uw \end{pmatrix}.$$

Combining we see

$$(L_+)^2\begin{pmatrix} v \\ v \end{pmatrix} = \begin{pmatrix} \partial_x^2 v - 4u\partial_x^{-1} u\partial_x v \\ \partial_x^2 v - 4u\partial_x^{-1} u\partial_x v \end{pmatrix} \equiv \begin{pmatrix} \mathscr{L} v \\ \mathscr{L} v \end{pmatrix}.$$

For any even power of L_+ we get two incompatible equations for u. If A_0 contains only odd powers, the equation (B10) is just

$$u_t = -\partial_x f(\mathscr{L})u$$

(i.e., the general member of the modified KdV hierarchy).

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On the covariant differential of spin direction in the Finslerian deformation theory of ferromagnetic substances

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(Received 2 April 1981; accepted for publication 30 July 1981)

In the Finslerian deformation theory of ferromagnetic substances, each point (x) is endowed with the unit vector (y) called the spin and the line-element (x,y) is taken as the independent variable. The length of y is normalized at each point, so that the direction of y alone is noticed. This is the so-called spin direction. In the case of the magnetization state, each vector y rotates to become parallel, in a Euclidean sense (not a Finslerian sense), to the direction of an applied magnetic field and the magnetostriction occurs there. Within the framework of Finsler geometry, this Euclidean "parallelism" of y cannot be grasped by the ordinary covariant differential of y (i.e., Dy), so that a new one (i.e., δy) must be introduced, which is nothing but the covariant differential of spin direction. Up to now, however, the geometrical meaning of δy and the relation between δy and Dy have not yet been clarified, so that these problems will be considered in this paper.

PACS numbers: 03.40. – t; 03.50.Kk

1. INTRODUCTION

In the (three-dimensional) continuum mechanics of ferromagnetic substances,[1] each point $x\,(=x^i;\ i=1,2,3)$ is endowed, at some macroscopic stage, with the vector $y\,(=y^j;\ j=1,2,3)$ called the magnetization vector or the spin, which embodies the magnetic moment per unit mass. From the standpoint of applied geometry,[2,3] if the pair (x,y) or the line-element (x,y) is chosen as the independent variable, instead of the point (x) alone, then there arises the Finslerian deformation theory of ferromagnetic substances, where some interesting physical features depending on y, such as magnetostriction, etc., are considered in terms of Finsler geometry (cf. Refs. 2 and 3). Usually, the length of the vector y, that is, the magnitude of spin is considered constant at each point and is prescribed as $\delta_{ij}y^iy^j=1$ (δ_{ij} is the Kronecker delta) by adopting proper units, so that only the direction of y is noticed. This is the so-called spin direction. In this paper, the words "vector y" and "spin direction" will be used equivalently for the sake of convenience. The vector y rotates around a point x and changes its direction continuously with position. These descriptions, therefore, are accepted for magnetically saturated media at temperatures significantly lower than the Curie temperature.[1,4]

Now, when an external magnetic field is applied to magnetize the ferromagnetic substance, each vector y rotates to become parallel to the direction of the applied field and neighboring vectors $\{y\}$ become parallel to each other in a Euclidean sense, not a Finslerian sense (cf. Ref. 4). Therefore, in this magnetization state, the "parallelism" of y is Euclidean, not Finslerian. Since the Finslerian parallelism of y is, of course, represented by the ordinary Finslerian covariant differential of y, i.e., Dy [see (2.2)], the above-mentioned Euclidean parallelism of y cannot be grasped by Dy. Therefore, in order to consider this Euclidean "parallelism" in the framework of Finsler geometry, it is necessary to introduce a new covariant differential of y (i.e., δy) different from the ordinary one (i.e., Dy). This δy [see (2.3)] is nothing else than the covariant differential of spin direction.[2] In Amari's theory,[2] δy is stipulated as $\delta y^i=Dy^i+\alpha y^i$, where α is a scalar, but this form has no significant geometrical meaning, due to the term αy^i, as will be explained in Sec. 4.

Moreover, in the magnetization state, since the parallelism of y is Euclidean, the Euclidean length of y (i.e., $\delta_{ij}y^iy^j=1$) is preserved invariant at each point under the "parallelism" δy, that is, the metric conditions $\delta\,\delta_{ij}=0$ [see (2.4)] hold good under the parallel displacement $\delta y=0$. In other words, it may be said that the covariant differential or the connection δ is caused to be metrical for the metric tensor δ_{ij}. Here, let the ordinary (or the originally introduced) Finslerian metric tensor be denoted by $g_{ij}(x,y)\ (\neq\delta_{ij})$. This Finslerian metric tensor g_{ij} is supposed, from the standpoint of the Finslerian deformation theory of ferromagnetic substances,[2,3] to be introduced from the beginning in order to govern the whole deformation field, although the spin direction (y) itself in the magnetization state is treated as a Euclidean quantity obeying the Euclidean parallelism δ. Then, the Finslerian length of y is given by $(g_{ij}y^iy^j)^{1/2}$, which is preserved invariant under the parallelism Dy, that is, the metric conditions $Dg_{ij}=0$ [see (2.5)] hold good under the parallel displacement $Dy=0$. In short, it may be said that in the magnetization state, there exist two different kinds of metrical connections δ and D for the two different kinds of metric tensors δ_{ij}, and g_{ij} respectively. Therefore, $D\delta_{ij}\neq0$ even if $\delta\delta_{ij}=0$ (resp., $\delta g_{ij}\neq0$ even if $Dg_{ij}=0$). These relations will be used to determine the relation between δy and Dy in Sec. 4.

It seems to the author that the introduction of $\delta y\ (\neq Dy)$ is inevitable whenever the deformation theory of the so-called oriented media is treated by means of Finsler geometry. However, the geometrical meaning of δy and the relation between δy and Dy have not yet been clarified, so far as the author knows (cf. Refs. 2 and 3). So these problems will be considered in this paper.

 0022-2488/81/122831-04$01.00

2. ON THE COVARIANT DIFFERENTIAL OF SPIN DIRECTION—I

Now, in general, the independent variable of the Finslerian field becomes the line-element (x,y), instead of the point (x), where the vector y $(=y^j; j=1,2,3)$ denotes the tangent vector at each point $x(=x^i; i=1,2,3)$ and represents physically the internal variable, such as the spin, associated with each point.[2,3,5,6] As the internal variable, the vector y shows its own intrinsic behavior, which geometrically appears above the surface as the intrinsic transformation or parallelism (i.e., parallel displacement) such as the above-mentioned δy different from the ordinary covariant differential of y (i.e., Dy). As is understood from the discussion in Sec. 1, this new parallelism δy $(\neq Dy)$, i.e., the covariant differential of spin direction must be introduced in order to preserve the Euclidean length of y (i.e., $\delta_{ij}y^iy^j=1$) invariant under the parallelism δy, that is, in order that the metric conditions $\delta\delta_{ij}=0$ be satisfied under the parallel displacement $\delta y=0$. These situations will be explained in more detail in this section.

Now, the ordinary (or the originally introduced) covariant differential of an arbitrary vector, say $X(=X^i)$, is expressed by, as usual,[7-9]

$$DX^i = dX^i + \Gamma^i_{kj}X^k dx^j + C^i_{kj}X^k dy^j, \tag{2.1}$$

where Γ and C denote the ordinary Finslerian coefficients of connection, which are, of course, functions of (x,y). These quantities Γ and C are combined with the Finslerian metric tensor $g_{ij}(x,y)$ by the metric conditions $Dg_{ij}=0$ [Eqs. (2.5)]. From the standpoint of applied geometry,[2,3] the deformation process itself is represented by the coordinate transformation, so that g_{ij}, Γ, and C are all determined by the deformation under some convenient conditions, because they are prescribed by their own coordinate transformations. When we put $X=y$ in (2.1), we can obtain

$$Dy^i = dy^i + \Gamma^i_{kj}y^k dx^j + C^i_{kj}y^k dy^j$$
$$(=A^i_j dy^j + B^i_j dx^j), \tag{2.2}$$

where we have put $A^i_j=\delta^i_j + C^i_{kj}y^k$ and $B^i_j=\Gamma^i_{kj}y^k$, but we have not assumed, in contrast to the Cartan's theory of Finsler spaces,[7] such homogeneity conditions as $C^i_{kj}y^k=0$ from a general viewpoint. Thus (2.2) represents the ordinary Finslerian parallelism of y.

In the Cartan's theory of Finsler Spaces,[7] the metric tensor $g_{ij}(x,y)$ is introduced through the so-called fundamental function $L(x,y)$, which is assumed to be positively homogeneous of degree 1 with respect to y, as follows: $g_{ij}=\frac{1}{2}\partial^2L^2/\partial y^i\partial y^j$ (or $L^2=g_{ij}y^iy^j$), which becomes positively homogeneous of degree 0 in y. In the case of ferromagnetism,[2-4] g_{ij} becomes an even function of y and represents the strain including the magnetostriction. Further, the relation $C^i_{kj}=C^i_{jk}$ is assumed in the Cartan's theory, so that from the metric conditions (2.5), C^i_{jk} is determined by $C^i_{jk}=\frac{1}{2}g^{il}(\partial g_{lj}/\partial y^k)=\frac{1}{4}g^{il}(\partial^3L^2/\partial y^l\partial y^j\partial y^k)$, which becomes positively homogeneous of degree -1 in y and as a result, such homogeneity conditions as $C^i_{jk}y^j=C^i_{jk}y^k=0$ hold good. In our case, however, these homogeneity conditions are not assumed from a general viewpoint [see (2.2) and (2.3)]. Of course, it is needless to say that the introduction of δy $(\neq Dy)$ itself is very different from the Cartan's theory.

From our standpoint, mentioned in Sec. 1, the covariant differential of spin direction (i.e., δy) cannot be obtained by Dy [see (2.2)], but requires such a newly-introduced formula as

$$\delta y^i = dy^i + \Delta^i_{kj}y^k dx^j + E^i_{kj}y^k dy^j$$
$$(=P^i_j dy^j + Q^i_j dx^j), \tag{2.3}$$

where the new Finslerian coefficients of connection Δ and E are assumed to be different from Γ and C, respectively, and we have put $P^i_j=\delta^i_j+E^i_{kj}y^k$ and $Q^i_j=\Delta^i_{kj}y^k$. (The relations between δy and Dy, and also (Δ,E) and (Γ,C) will be obtained in Sec. 4.) Corresponding to (2.2), such homogeneity conditions as $E^i_{kj}y^k=0$ are also not assumed, because there exists no physical reason to assume them from a general viewpoint (cf. Ref. 2).

In this case, there exist two different parallelisms or connections $(\delta y\neq Dy)$, so that, inevitably, $Dy\neq0$ even if $\delta y=0$, (resp., $\delta y\neq0$ even if $Dy=0$). As for the parallelism or the connection δ, since the Euclidean length of y (i.e., $\delta_{ij}y^iy^j=1$) must be preserved under the parallelism δy, the metric conditions $\delta\delta_{ij}=0$ are required to hold good under the parallel displacement $\delta y=0$ [see (2.3)], i.e.,

$$\delta\delta_{ij} = d\delta_{ij} - \Delta^l_{ik}\delta_{lj}dx^k - \Delta^l_{jk}\delta_{il}dx^k$$
$$- E^l_{ik}\delta_{lj}dy^k - E^l_{jk}\delta_{il}dy^k = 0. \tag{2.4}$$

On the other hand, the ordinary (or the originally-introduced) Finslerian metric tensor g_{ij} must satisfy the following metric conditions [see (2.1)] to preserve the Finslerian length of y (i.e., $g_{ij}y^iy^j$) invariant under the parallel displacement $Dy=0$:

$$Dg_{ij} = dg_{ij} - \Gamma^l_{ik}g_{lj}dx^k - \Gamma^l_{jk}g_{il}dx^k$$
$$- C^l_{ik}g_{lj}dy^k - C^l_{jk}g_{il}dy^k = 0. \tag{2.5}$$

Then, there exist two different metrical connections δ and D for two different metric tensors δ_{ij} and g_{ij}, respectively. Therefore, it is also true that $D\delta_{ij}\neq0$ even if $\delta\delta_{ij}=0$ (resp., $\delta g_{ij}\neq0$ even if $Dg_{ij}=0$), as has already been postulated. These relations will be used to determine the relation between δy and Dy in Sec. 4.

Now, when the intrinsic parallelism of y, i.e., δy given by (2.3) is taken into account, the originally-introduced spatial structure of the field represented by (2.1) must be changed as follows:

$$DX^i = dX^i + \Theta^i_{kj}X^k dx^j + F^i_{kj}X^k\delta y^j, \tag{2.6}$$

where $\Theta^i_{kj}=\Gamma^i_{kj}-N^l_jC^i_{kl}$, $F^i_{kj}=(P^{-1})^l_jC^i_{kl}$ and $N^l_j=Q^m_j(P^{-1})^l_m$. Equation (2.6) is obtained as follows: First, from (2.3), dy is obtained by $dy^j=(P^{-1})^j_i(\delta y^i-Q^i_k dx^k)$ under the assumption that P is nonsingular. Second, substituting this dy into (2.1), we can obtain (2.6). From (2.6), the following two kinds of covariant derivatives are defined[7-9]:

$$DX^i = (X^i{}_{|j})dx^j + (X^i|_j)\delta y^j;$$
$$X^i{}_{|j} = \frac{\delta X^i}{\delta x^j} + \Theta^i_{kj}X^k, \tag{2.7}$$
$$X^i|_j = \frac{\delta X^i}{\delta y^j} + F^i_{kj}X^k,$$

where $\delta/\delta x^j = \partial/\partial x^j - N^l_j \partial/\partial y^l$ and $\partial/\partial y^j = (P^{-1})^l_j \partial/\partial y^l$. From (2.7), three kinds of curvature tensors and five kinds of torsion tensors can be introduced through the so-called Ricci identities, but they are omitted here for the sake of simplicity [cf. (3.2) and Ref. 9]. Of course, the metric conditions $g_{ij|k} = 0$ and $g_{ij}|_k = 0$ hold good because $Dg_{ij} = 0$. It should be noted here that the covariant derivatives of y determined by (2.7) are given by $y^i{}_{|j} = -N^i_j + \Theta^i_{kj} y^k \neq 0$ and $y^i|_j = \delta^i_j$. The fact that $y^i{}_{|j} \neq 0$ is caused by the prescription $\delta y \neq Dy$, which is also different from the Cartan's theory.[7]

Thus, it is found that the covariant differential of spin direction δy is given by (2.3) and the whole spatial structure of the field itself is represented by (2.6) and (2.7). It should also be remarked that these considerations are generally applicable to any Finslerian field theory, where the vector y plays physically a role of internal variable associated with each point and δy means the inherent law of y.[5,6,10]

3. ON THE COVARIANT DIFFERENTIAL OF SPIN DIRECTION—II

The covariant differential of spin direction obtained above, i.e., δy, may be regarded geometrically as the intrinsic parallelism of y. In our case, when the condition $\delta y = 0$ holds good, the vector y is displaced parallel to itself under the Euclidean parallelism δ, and the metric conditions $\delta\,\delta_{ij} = 0$ hold good. On the other hand, δy may physically be compared, in a certain sense, to the inherent law of y, so that the state in which $\delta y = 0$ holds good may be likened to an "exciting" state where the inherent law of y is satisfied.[10] Therefore, in our case, this state corresponds to the magnetization state of the magnetically-saturated medium,[1,4] because each vector y rotates to become parallel to the direction of an applied magnetic field and neighboring vectors $\{y\}$ become parallel to each other in a Euclidean sense (i.e., $\delta y = 0$), and the Euclidean length of y (i.e., $\delta_{ij} y^i y^j = 0$) is kept constant, that is, the metric conditions $\delta\,\delta_{ij} = 0$ hold good.

Now, when the condition $\delta y = 0$ holds good, (2.6) and (2.7) are reduced to

$$DX^i = dX^i + \Theta^i_{kj} X^k dx^j = (X^i{}_{|j}) dx^j, \tag{3.1}$$

from which the curvature tensor (R) and the torsion tensors (T,S) are introduced through the following Ricci identity:[9]

$$\begin{aligned} &X^i{}_{|j|k} - X^i{}_{|k|j} = R^i{}_{ljk} X^l - T^l_{jk} X^i{}_{|l} - S^m_{jk} P^l_m X^i|_l; \\ &R^i{}_{ljk} = \mathfrak{A}_{jk} \left\{ \frac{\delta \Theta^i_{lj}}{\delta x^k} + \Theta^i_{mk} \Theta^m_{lj} \right\} + C^i_{lm} S^m_{jk}, \\ &T^i_{jk} = \mathfrak{A}_{jk} \{ \Theta^i_{jk} \}, \\ &S^i_{jk} = \mathfrak{A}_{jk} \left\{ \frac{\delta N^i_j}{\delta x^k} \right\}, \end{aligned} \tag{3.2}$$

where the symbol $\mathfrak{A}_{jk}$ means interchange of indices j,k and subtraction.[9] These tensors appear owing to the condition $Dy \neq 0$ (i.e., $y^i{}_{|j} \neq 0$ and $y^i|_j \neq 0$), so that they, especially the curvature tensor R, reflect truly the difference between δy and Dy (see also below).

Furthermore, as is usually assumed in most physical cases, if y is given by a function of x from the condition $\delta y = 0$, then the equation $\partial y^i/\partial x^j = -N^i_j$ derived from (2.3) becomes completely integrable and as the result, one kind of torsion S of (3.2) disappears.[9] Therefore, in this magnetization state, the torsion tensor T and the curvature tensor R survive, the former being regarded as the magnetostriction caused by the rotation of y (cf. Ref. 2), while the latter is related, for example, to such a second-order effect as the change of elastic coefficient due to the magnetostriction.[4] In Amari's theory,[2] the Finslerian coefficients of connection Γ and C are uniquely determined by the deformation under the assumption that the deformation is separated into the x- and y-dependent parts (i.e., under the crystallographic deformation), so that the teleparallelism condition, i.e., $R = 0$, is further assumed and consequently, only the torsion tensor T survives.

By the way, when the condition $Dy = 0$ holds good (but $\delta y \neq 0$), each vector y takes its intrinsic direction at each point and neighboring vectors $\{y\}$ become parallel to each other in a Finslerian sense (not a Euclidean sense). Therefore, this state may be compared, to some extent, to the spontaneous magnetization state,[4] whose spatial structure is governed by the following formulas, corresponding to (3.1):

$$\begin{aligned} &DX^i = dX^i + G^i_{kj} X^k dx^j = (X^i{}_{\|j}) dx^j, \\ &X^i{}_{\|j} = \left(\frac{\partial}{\partial x^j} - M^l_j \frac{\partial}{\partial y^l} \right) X^i + G^i_{kj} X^k, \end{aligned} \tag{3.3}$$

where $G^i_{kj} = \Gamma^i_{kj} - M^l_j C^i_{kl}$ and $M^l_j = B^m_j (A^{-1})^l_m$. Equation (3.3) is obtained as follows: First, from (2.2) and $Dy = 0$, dy is obtained by $dy^j = -M^j_k dx^k$ under the assumption that A is nonsingular. Second, substituting this dy into (2.1), we can get (3.3). In this case, by taking account of the Ricci identity derived from (3.3) corresponding to (3.2) and then putting $X = y$, it is found that the curvature tensor corresponding to R of (3.2) vanishes, if y is given by a function of x through the condition $Dy = 0$, but the torsion tensor corresponding to T appears in general, which means, for this state, the spontaneous magnetostriction.[4]

Thus, it is understood from the above that in the magnetization state in which the condition $\delta y = 0$ holds good, the spatial structure is governed by (3.1) and there appear the tensors introduced by (3.2).

4. ON THE RELATION BETWEEN δy AND Dy

As has already been mentioned in Secs. 1 and 2, in the Finslerian deformation theory of ferromagnetic substances,[2,3] two different kinds of metrical connections δ and D are inevitably introduced for two different kinds of metric tensors δ_{ij} and g_{ij}, respectively [see Eqs. (2.4) and (2.5)], in order to take the Euclidean parallelism δy in the framework of Finsler geometry and reflect it in the whole spatial structure of the deformation field itself. But the relation between δy and Dy has not yet been clarified, so that this problem will be considered in this section.

First, we recall the following fact: The newly introduced parallelism, or connection δ, is caused to be metrical (under $\delta y = 0$) for the metric tensor δ_{ij}, i.e., $\delta\,\delta_{ij} = 0$ [Eq. (2.4)], while the ordinary (or the originally-introduced) con-

nection D is metrical (under $Dy = 0$) for the metric tensor g_{ij}, i.e., $D\,g_{ij} = 0$ [Eq. (2.5)]. As a result $\delta\,g_{ij} \neq 0$ even if $\delta\,\delta_{ij} = 0$ (resp., $D\delta_{ij} \neq 0$ even if $Dg_{ij} = 0$), and also $D\delta_{ij} \neq 0$ even if $\delta\,\delta_{ij} = 0$, (resp., $\delta\,g_{ij} \neq 0$ even if $D\,g_{ij} = 0$).

This last relation is very useful for our purpose, because if we take account of the Kawaguchi's theorem,[11] then we can obtain one relation between δy and Dy from it. Kawaguchi's theorem[11] supplies a general method to make a nonmetrical connection metrical. From the standpoint of this theorem, the relation that $\delta\,\delta_{ij} = 0$ but $D\,\delta_{ij} \neq 0$ (resp., $D\,g_{ij} = 0$ but $\delta g_{ij} \neq 0$) may be reconsidered as follows: The connection δ may be regarded as a metrical connection for δ_{ij}, i.e., $\delta\,\delta_{ij} = 0$, derived from the nonmetrical one D, i.e., $D\delta_{ij} \neq 0$ (resp., the connection D may be regarded as a metrical connection for g_{ij}, i.e., $D\,g_{ij} = 0$, derived from the nonmetrical one δ, i.e., $\delta\,g_{ij} \neq 0$). Therefore, applying Kawaguchi's theorem to our case, we can obtain the following relation, neglecting arbitrariness[11]:

$$\delta y^i = Dy^i + H^i_{\ k} y^k; \quad H^i_{\ k} = \tfrac{1}{2}\delta^{il} D\delta_{lk}, \tag{4.1}$$

where $D\delta_{lk}$ is given by use of (2.5) (with $d\delta_{lk} = 0$) [resp.,

$$Dy^i = \delta y^i + K^i_{\ k} y^k; \quad K^i_{\ k} = \tfrac{1}{2} g^{il} \delta g_{lk}, \tag{4.2}$$

where δg_{lk} is obtained by use of (2.4)]. Then, the following relations can be obtained by inserting (2.2) and (2.3) into (4.1) [resp., (4.2)]:

$$\begin{aligned} \Delta^i_{\ kj} &= \Gamma^i_{\ kj} + \tfrac{1}{2}\delta^{il}(-\Gamma^m_{\ lj}\delta_{mk} - \Gamma^m_{\ kj}\delta_{lm}), \\ E^i_{\ kj} &= C^i_{\ kj} + \tfrac{1}{2}\delta^{il}(-C^m_{\ lj}\delta_{mk} - C^m_{\ kj}\delta_{lm}). \end{aligned} \tag{4.3}$$

Respectively,

$$\begin{aligned} \Gamma^i_{\ kj} &= \Delta^i_{\ kj} + \tfrac{1}{2} g^{il}\left(\frac{\partial g_{lk}}{\partial x^j} - \Delta^m_{\ lj} g_{mk} - \Delta^m_{\ kj} g_{lm}\right), \\ C^i_{\ kj} &= E^i_{\ kj} + \tfrac{1}{2} g^{il}\left(\frac{\partial g_{lk}}{\partial y^j} - E^m_{\ lj} g_{mk} - E^m_{\ kj} g_{lm}\right). \end{aligned} \tag{4.4}$$

With the aid of (4.3) or (4.4), if Γ and C are determined first by the deformation under consideration, then Δ and E are determined, and vice versa (cf. Ref. 2). From (4.3), such quantities as P and Q of (2.3) and then Θ and F of (2.6) and (2.7) can also be written in terms of Γ and C, respectively. [From (4.4), such quantities as A and B of (2.2) and then G of (3.3) can also be written in terms of Δ and E.] But they become very complicated due to the term P^{-1} or A^{-1}, so that they are omitted here for simplicity's sake.

Thus, the relation between δy and Dy has been clarified. And it is clearly understood that the relation (4.1) or (4.2) embodies faithfully the fact that $Dy \neq 0$ even if $\delta y = 0$, and vice versa.

In Amari's theory,[2] the covariant differential of spin direction, i.e., δy is introduced in the form $\delta y^i = Dy^i + \alpha y^i$. In comparison with (4.1), the scalar α is, in our terms, formally determined as $\alpha = \delta_{im} y^m H^i_{\ k} y^k$ by virtue of the relation $\delta_{ij} y^i y^j = 1$. But Amari's operator δ itself cannot be applied to any tensor such as δ_{ij} because of the term αy^i, so that geometrical considerations like ours cannot be developed; in particular Kawaguchi's theorem cannot be used. Therefore, it seems to the author that Amari's definition of δy does not have any significant geometrical meaning.

5. CONCLUSIONS

Some physico-geometrical remarks have been made on the covariant differential of spin direction (i.e., δy) within the Finslerian deformation theory of ferromagnetic substances:[2,3] First, δy itself is given by (2.3), which is premised to be different from the ordinary covariant differential of y (i.e., Dy) given by (2.2); when δy is taken into account, the whole spatial structure of the Finslerian field is represented by (2.6) and (2.7); in the magnetization state in which the condition $\delta y = 0$ holds good, the spatial structure is governed by (3.1); one relation between δy and Dy is given by (4.1) or (4.2); etc.

It seems to the author that the introduction of δy ($\neq Dy$) and the relation between δy and Dy have not been considered seriously, even in the theory of fields in Finsler spaces.[5,6,10] This is a motivation for this paper. Finally, the author would like to insist again that this kind of theory would become effective whenever the deformation theory of the so-called oriented media was treated by means of Finsler geometry.

ACKNOWLEDGMENTS

The author would like to thank Professor Y. Takano and Professor S. Watanabe for valuable discussions.

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Signals and discontinuities in general relativistic nonlinear electrodynamics

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(Received 6 January 1981; accepted for publication 27 March 1981)

A theory of nonlinear electrodynamics in an arbitrary curved space–time is developed from the fundamental action functional for a charged perfect fluid. The equations for small perturbations on a fixed nonlinear background are then the initial point for a comprehensive study of the characteristic surfaces. The essential distinctions between linear and nonlinear electrodynamic interactions under the influence of gravitation are exhibited. Discontinuities in the first derivatives of small perturbations are encountered (1) which may be of general algebraic types for both the electrodynamic and gravitational fields and (2) which may have spacelike propagation. A specific set of constraints which would permit the propagation of these extraordinary radiative fronts is presented. If the physical organization of a particular problem is presumed to be sufficiently sensitive to the nonlinear nature of the dynamical interactions, then the application of traditional causal concepts may be unreliable when intuition derived from Maxwellian electrodynamics with noninteracting photons is anticipated to provide event horizons.

PACS numbers: 03.50.Kk, 04.20.Fy

1. INTRODUCTION

This paper has two basic objectives. The first is to present a compact covariant exposition of nonlinear electrodynamics (NLE) in a curved space–time (i.e., the dynamics of the Einstein–Born–Infeld equations with a general structure function), investigating the algebraic aspects of the theory by spinorial techniques. The second is to offer a comprehensive study of the characteristic surfaces of such a system, demonstrating the essential distinctions between the linear and nonlinear electrodynamic cases.

The actual content of the work is a generalization of Ref. 1. drawing extensively from the calculations presented in Ref. 2. The paper continues the sequential study of NLE with its vast literature[3–13] initiated by Born and Infeld. Because of the similarities between Refs. 1 and 13, the results may also be thought of as an extension of those of Boillant. Recently these ideas of NLE have been found of interest even in supersymmetric theories.[14]

There are two physical approaches to the theory. The first is to seek, via nonlinearity, a structurally self-consistent classical electrodynamics with a finite point charge inertia which is free of the conceptual difficulties related to the divergences which plague the linear theory. Within this approach, with a sensible structure function of invariants, NLE is capable of fulfilling all common sense requirements (like, e.g., the correct transformation properties for finite conserved quantities of a point charge) in contrast to other variants, including those with extended sources, higher derivatives, form factors, etc., each of which retains some incompatibility. Unfortunately, the shape of the structure function remains remarkably arbitrary, which handicaps specific physical predictions from the theory. This is the main reason for the limited interest in these matters in general theoretical physics. The second approach regards NLE as a variety of phenomenological quantum electrodynamics (QED) in the limit of high occupation numbers. The structure function is selected such that the QED predictions concerning the scattering of light by light are reproduced classically by the NLE. Of particular interest is the structure function of Schwinger,[15] which accounts for an infinite ladder of quantum processes. Our motivations are closer to the second of these options.

If electromagnetic fields in curved space–times are critical to the early evolution of the universe or for the dynamics of collapsing objects near singularity limits, then it is natural to expect the corresponding QED dependent processes will affect the physics. Hence, NLE provides a simple tool for evaluating possible implications closer to physical reality. It is rather naive to anticipate that classical Maxwellian electrodynamics with noninteracting photons can reliably represent such extremal conditions. Consequently, it is interesting to study the nature of causal signals within Einstein–Born–Infeld dynamics. The original Einstein construction of causal cones is related to light or, more specifically, to the surfaces along which discontinuities of the first derivatives of the electromagnetic field (characteristic surfaces) of linear electrodynamics are propagated. Light rays are then understood as bicharacteristic lines. This identification forms the foundation of special relativity, and without alteration it is extrapolated into the realm of general relativity. In fact, in general relativity, when a linear Maxwellian field is present, its characteristics do coincide with the Einsteinian $g_{\mu\nu}$ cone. This, however, will not be the case when NLE governs electromagnetic phenomena. This result permits the reinterpretation of the standard characteristic of general relativity, the eiconal equation $g^{\mu\nu}S_{,\mu}S_{,\nu} = 0$, which is a major objective of this paper. It is not unreasonable to assume that the introduction of other forms of nonlinear interactions (e.g., fluid dynamic or Yang–Mills fields) would produce analogous results.

Formally, the paper is organized such that Sec. 2 contains the generation of the dynamic equations for a perfect charged fluid, containing a nonlinear electrodynamic interaction within a curved space–time, by variations of the fundamental action. The structure equations which contain the distinction between the linear and nonlinear electrodynamic

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 0022-2488/81/122835-14$01.00

cases are introduced. Section 3 provides the conversion of the equations into their spinor counterparts and reviews the algebraic properties of the electromagnetic field tensors critical to the evaluation of the characteristic surfaces. There is also a brief discussion of how the NLE presented can be interpreted as analogous to more conventional electrodynamics within a medium. The entire self-consistent system is linearized by standard first perturbation techniques and the "jump" expressions satisfied by the discontinuities in the first derivatives of the field variables are given in Sec. 4. Section 5 demonstrates how the system reduces identically to the standard results in the linear electrodynamic limits. In particular, the algebraic investigation indicates that in the linear limit only null characteristic surfaces permit the existence of nontrivial jumps. Section 6 classifies in detail the necessary conditions for the jump expressions for the many possible characteristics determined by the structure function in the NLE case. Dependent upon the nonlinearity, the results indicate that the discontinuities of both the gravitational and electromagnetic fields may be of algebraically general types with respect of the Einsteinian metric. The Einsteinian local null cone is physically identified only with the propagation of pure gravitational radiative fronts, and there exist nonlinearly interacting massless fields (including the elctrodynamic) whose propagation may be associated with causal cones both interior and exterior to the Einsteinian null cone. Assuming there exist physically reasonable nonlinear structure functions, satisfying a rather simple set of conditions, these different cones which allow causal influence certainly do no coincide. The distinguished rate of propagation of discontinuities in conformal curvature alters the local measurement of time and thereby changes our traditional view of the propagation of linear electrodynamic fronts as the only provider of a causal horizon for an event. The metric properties for each form of characteristic surface are then cataloged in Sec. 7, and finally Sec. 8 concludes by displaying the algebraic types of jumps in tabular form.

2. THE DYNAMIC EQUATIONS

The relevant dynamic equations are evaluated by variations of the action functional

$$\mathscr{A} := \int_{\Omega} d^4x\,(-g)^{1/2}(\mathscr{L}_F + \mathscr{L}_E + \mathscr{L}_I + \mathscr{L}_G), \quad (2.1)$$

where the infinitesimal four-volume element $d^4x(-g)^{1/2}$ is invariant under nonsingular coordinate transformations within a Riemannian background space-time V_4 represented by the metric $g_{\mu\nu}$ with signature $(+\ +\ +\ -)$ and determinant g. The associated Lagrangians correspond to the fluid $\mathscr{L}_F$, the nonlinear electrodynamic field $\mathscr{L}_E$, the interaction between the fluid and field $\mathscr{L}_I$, and the background gravitational field $\mathscr{L}_G$, respectively. The line integrals are understood to be taken along the world line of fluid particles between the points of intersection with two spacelike three-surfaces bounding the domain Ω of variation.

Assuming there exists a known equation of state such that the energy density is given by $\epsilon = \epsilon(n,s)$, where n denotes the particle density and s the entropy density of a fluid point, the fluid flow may be characterized by (1) an Eulerian velocity $u^\mu(x^\nu)$ defined for every event $P(x^\nu)$ situated on its world trajectory, (2) the specific volume $V = 1/n$, and (3) the phenomenologic temperature T and pressure p encountered. These hydrodynamic variables are measured with respect to a local rest frame. The velocity is normalized such that $u^\mu u_\mu = -1$. Since the fluid is isotropic and frictionless, entropy is conserved. Therefore,

$$\text{a)}\ u^\alpha s_{,\alpha} = 0$$

and (2.2)

$$\text{b)}\ (nu^\alpha)_{;\alpha} = 0.$$

The first and second laws of thermodynamics,

$$d\epsilon = nTds + [(\epsilon + p)/n]dn, \quad (2.3)$$

are postulated. Associated with such a fluid is the Lagrangian density

$$\mathscr{L}_F = -\epsilon(n,s). \quad (2.4)$$

The nonlinear electrodynamic field is represented by two skew field tensors $f_{\mu\nu}$ and $P_{\mu\nu}$, which are interrelated through a single relation designated as the "structure" equation. The existence of a potential A satisfying the Faraday field equation

$$f_{\mu\nu} = A_{\mu;\nu} - A_{\nu;\mu} \quad (2.5)$$

is assumed, yielding the electrodynamic Lagrangian

$$\mathscr{L}_E = -(1/4\pi)[\tfrac{1}{2}f_{\mu\nu}P^{\mu\nu} - H(P,\breve{Q})]. \quad (2.6)$$

The "structure function" $H = H(P,\breve{Q})$, whose arguments[16]

$$P := \tfrac{1}{4}P_{\mu\nu}P^{\mu\nu} \text{ and } \breve{Q} := \tfrac{1}{4}P_{\mu\nu}\breve{P}^{\mu\nu} \quad (2.7)$$

are invariant (scalar) and pseudoinvariant,[17] respectively, is a real Hamiltonian whose functional form is intentionally left unspecified. For linear electrodynamics $H = P$, but for nonlinear electrodynamics H must only conform to a couple of general conditions. One expects for the weak field ($P,\breve{Q}$ small) limit that nonlinear effects will become negligible:

$$\text{correspondence} \rightarrow H(P,\breve{Q}) = P + O(P^2,\breve{Q}^2)$$
$$\Rightarrow H_P(0,0) = 1. \quad (2.8)$$

If parity is conserved, then under coordinate transformations with negative Jacobian, where $\breve{Q}$ transforms into $-\breve{Q}$, H must remain invariant

$$\text{parity conservation} \rightarrow H(P,\breve{Q}) = H(P,-\breve{Q}), \quad (2.9)$$

which is equivalent to $H = H(P,\breve{Q}^2)$. Condition (2.9) is less essential than (2.8), since one could consider systems with parity violating weak interactions in a quantized theory. However, in this work, both restrictions (2.8) and (2.9) are presumed satisfied. Additionally, the conservation of charge density ρ,

$$(\rho u^\alpha)_{;\alpha} = 0, \quad (2.10)$$

is required.

The interaction between the fluid and the nonlinear electrodynamic field is provided by the minimal coupling Lagrangian density

$$\mathscr{L}_I = A_\mu J^\mu, \quad (2.11)$$

where $J^\mu = \rho u^\mu$ denotes the electric current density. Notice

that the expressions determining the inertia of the fluid (2.4) and the coupling with the electromagnetic field (2.11) are identical to those of linear electrodynamics.

The gravitation field equations are deduced from the conventional Lagrangian density of Einsteinian gravity,

$$\mathscr{L}_G = (1/16\pi)(R + 2\lambda), \tag{2.12}$$

written in gravitational units ($G =$ gravitational constant $= 1 =$ velocity of light $= c$), with scalar curvature R and cosmological constant λ.[18] Restricting this work to special relativity (in general coordinates) by submitting the metric $g_{\mu\nu}$ to the condition of vanishing Riemann tensor ($R^{\alpha}{}_{\beta\gamma\delta} = 0$) yields the results previously given in Ref. 1.

The dynamic equations are derived from the overall action $\mathscr{A}$ of (2.1) accounting for (2.4), (2.6), (2.11), and (2.12) by executing the variations and extremalizing with respect to (1) the Lagrangian trajectories (δx^{μ}), (2) the potential (δA_{μ}), (3) the field $P_{\mu\nu}$ regarded as Lagrange multiplier ($\delta P_{\mu\nu}$), (4) the metric ($\delta g_{\mu\nu}$), and (5) the connections $\Gamma^{\mu}{}_{\nu\lambda}$ considered as independent of the metric ($\delta\Gamma^{\mu}{}_{\nu\lambda}$) (according to the principle of Palatini). The process must be consistent with the subsidiary conservation conditions (2.2) and (2.10), and constrained by null variations on the boundary $\partial\Omega$ of the region Ω. Performing the extremalizations, the following equations of evolution of the perfect fluid system with nonlinear electrodynamic and gravitational fields are evaluated. The details are found in Ref. 2.

$$\delta\mathscr{A}/\delta\Gamma^{\alpha}{}_{\mu\nu} = 0 \rightarrow \mathscr{J}^{\mu\nu}{}_{;\alpha} - \delta^{\nu}{}_{\alpha}\mathscr{J}^{\mu\beta}{}_{;\beta} = 0 \leftrightarrow g_{\mu\nu;\alpha} = 0, \tag{2.13}$$

where $\mathscr{J}^{\mu\nu} := (-g)^{1/2}g^{\mu\nu}$. Consequently, the appropriate connection for the metric is that of Levi-Civita ($\{^{\alpha}_{\beta\gamma}\} = \Gamma^{\alpha}{}_{\beta\gamma}$). The equations of motion (Lorentz equations) for the charged fluid are

$$\delta\mathscr{A}/\delta x_{\perp} = 0 \rightarrow T^{\mu\nu}{}_{;\nu} + f^{\mu}{}_{\nu}J^{\nu} = 0, \tag{2.14}$$

where $\delta x^{\nu} := \delta x^{\nu}{}_{\perp} + u^{\nu}\delta x_{\parallel}$ with $\delta x^{\nu}{}_{\perp}u_{\nu} = 0$ and the energy-momentum tensor is defined by $T^{\mu\nu} := pg^{\mu\nu} + (\epsilon + p)u^{\mu}u^{\nu}$. The electromagnetic field (Maxwell's) equations are

$$\delta\mathscr{A}/\delta A_{\mu} = 0 \rightarrow P^{\mu\nu}{}_{;\nu} = 4\pi J^{\mu}. \tag{2.15}$$

These equations are complemented by the Faraday equations (the existence of the potential), which express the necessary and sufficient conditions that $f_{\mu\nu}$ be a curl,

$$\check{f}^{\mu\nu}{}_{;\nu} = 0 \leftrightarrow f_{[\mu\nu;\lambda]} = 0 \leftrightarrow f_{\mu\nu} = A_{\mu,\nu} - A_{\nu,\mu}. \tag{2.16}$$

The structure equations (material equations)

$$\delta\mathscr{A}/\delta P^{\mu\nu} = 0 \rightarrow f_{\mu\nu} = 2\partial H/\partial P^{\mu\nu} = H_P P^{\mu\nu} + H_{\check{Q}}\check{P}^{\mu\nu} \tag{2.17}$$

are the counterparts of the Lorentz material equations in the classical electrodynamics of polarized media. Equations (2.15)–(2.17) give the physical interpretation and the evolution of the nonlinear electrodynamic field whose energy-momentum tensor is defined by

$$4\pi E^{\mu\nu} := -f^{\mu\lambda}P^{\nu}{}_{\lambda} + g^{\mu\nu}L \text{ with } L := -4\pi\mathscr{L}_E. \tag{2.18}$$

For a linear field, $H = P \rightarrow f_{\mu\nu} = P_{\mu\nu}$. Varying the metric, one obtains the gravitation equations (Einstein equations)

$$\delta\mathscr{A}/\delta g_{\mu\nu} = 0 \rightarrow G^{\mu\nu} = 8\pi(T^{\mu\nu} + E^{\mu\nu}) + \lambda g^{\mu\nu}, \tag{2.19}$$

where $G^{\mu\nu} := R^{\mu\nu} - \frac{1}{2}g^{\mu\nu}R$ is the Einstein tensor. The expression (2.19) and the geometric structure equations (Bianchi identities)

$$R^{\alpha\beta}{}_{[\gamma\delta;\lambda]} = 0 \tag{2.20a}$$

and

$$G^{\mu\nu}{}_{;\nu} = 0 \tag{2.20b}$$

govern the evolution of space-time and the motion of material contained within it. This essentially completes the system of dynamical equations. The conservation constraints (2.2) and (2.10) have been inherently imposed. When this system is restricted to special relativity, where the Riemann tensor vanishes, the total energy-momentum tensor is still divergenceless as (2.20b) implies, but now as the result of the translational invariance of the action.

Since the essential distinction between linear and nonlinear electrodynamics resides in the electromagnetic structure equations (2.17), it is informative from the outset to inquire about their inversion. When these equations can be inverted one may algebraically express $P_{\mu\nu}$ through $f_{\mu\nu}$, its dual, and the invariants

$$F := \tfrac{1}{4}f_{\mu\nu}f^{\mu\nu} \text{ and } \check{G} := \tfrac{1}{4}f_{\mu\nu}\check{f}^{\mu\nu}, \tag{2.21}$$

by the expression

$$P_{\mu\nu} = 2\,\partial L/\partial f^{\mu\nu} = L_F f_{\mu\nu} + L_{\check{G}}\check{f}_{\mu\nu}. \tag{2.22}$$

Hence $L = L(F,\check{G})$ is understood as a function of $f_{\mu\nu}$ depending on it throught the arguments F and $\check{G}$. The relations among invariants can be represented by a complex equation in either of the forms

$$F + \check{G} = (H_P + H_{\check{Q}})^2(P + \check{Q}) \tag{2.23a}$$

or

$$P + \check{Q} = (L_F + L_{\check{G}})^2(F + \check{G}). \tag{2.23b}$$

Thus, if (2.23a) can be inverted [i.e., $\partial(F,\check{G})/\partial(P,\check{Q}) \neq 0$] determining $P = P(F,\check{G})$ and $\check{Q} = \check{Q}(F,\check{G})$, then

$$L(F,\check{G}) = 2PH_P + 2\check{Q}H_{\check{Q}} - H. \tag{2.24}$$

Moreover, (2.22) substituted into the definition of L [(2.6) and (2.18)] implies

$$H(P,\check{Q}) = 2FL_F + 2\check{G}L_{\check{G}} - L. \tag{2.25}$$

The self-consistency of the theory is demonstrated by showing that the divergence of the total energy-momentum tensor, indicated in the special Bianchi identity (2.20b), vanishes. Sequentially, this is accomplished by applying the equations of Lorentz, Maxwell, and Faraday, the definition of the dual, the electromagnetic structure relation, the antisymmetry property of $P^{\mu\nu}$, and finally the definition of $E^{\mu\nu}$.

3. SPINOR FORM OF THE EQUATIONS

Since the classification of the characteristic surfaces is conveniently done in spinor formalism, the spinorial counterparts of the dynamic equations are now presented. Using the Hermitian Pauli matrices $g^{\mu}{}_{A\dot{B}}$, the self-dual spin tensor $S^{\mu\nu}{}_{AB}$, and its anti-self-dual complex conjugate $S^{\mu\nu}{}_{\dot{A}\dot{B}}$,[19] the spinorial images of all relevant objects may be defined in

the usual manner. The spinor covariant derivative operator is $\nabla_{A\dot{B}} := g^{\mu}{}_{A\dot{B}}\nabla_{\mu}$. For the symbols corresponding identically to those used previously, the equations of motion (2.14), Maxwell (2.15), and Faraday (2.16), respectively, become

$$u_{A\dot{A}}u^{S\dot{S}}\nabla_{S\dot{S}}p + \tfrac{1}{2}\nabla_{A\dot{A}}(\epsilon + p) + (\epsilon + p)u^{S\dot{S}}\nabla_{S\dot{S}}u_{A\dot{A}} = 2f_{AS}J^{S}{}_{\dot{A}} + 2f_{\dot{A}\dot{S}}J_{A}{}^{\dot{S}}, \tag{3.1}$$

$$\nabla^{S\dot{A}}P^{B}{}_{S} + \nabla^{B\dot{S}}P^{\dot{A}}{}_{\dot{S}} = 4\pi J^{B\dot{A}}, \tag{3.2}$$

$$\nabla^{S\dot{A}}f^{B}{}_{S} - \nabla^{B\dot{S}}f^{\dot{A}}{}_{\dot{S}} = 0 \leftrightarrow f_{AB} = -\nabla_{A}{}^{\dot{S}}A_{B\dot{S}} - \nabla_{B}{}^{\dot{S}}A_{A\dot{S}}, \tag{3.3}$$

complemented by the conservation of charge (2.10) $\nabla^{A\dot{B}}J_{A\dot{B}} = 0$. The electromagnetic structure (material) equations (2.17) and their inverses (2.22) are most conveniently written in their equivalent spinorial relations after the introduction of

$$Z := P + \check{Q} = 4P^{AB}P_{AB} \text{ and}$$
$$W := F + \check{G} = 4f^{AB}f_{AB} \tag{3.4}$$

and the respective complex conjugates as the independent invariants. We obtain

$$f_{AB} = 2H_{Z}P_{AB} \tag{3.5a}$$

and

$$P_{AB} = 2L_{W}f_{AB}, \tag{3.5b}$$

which are equivalent to

$$f_{AB} = (H_{P} + H_{\check{Q}})P_{AB} \tag{3.6a}$$

and

$$P_{AB} = (L_{F} + L_{\check{G}})f_{AB}. \tag{3.6b}$$

Moreover, (3.6) implies

$$(H_{P} + H_{\check{Q}})(L_{F} + L_{\check{G}}) = 1. \tag{3.7}$$

For the symmetric tensors, the trace is extracted before contracting each index independently with $\frac{1}{2}$ of the general Pauli matrices. The traceless energy-momentum tensor of the fluid is $F^{\mu\nu} := T^{\mu\nu} - \frac{1}{4}g^{\mu\nu}T^{\lambda}{}_{\lambda}$. Hence it has a spinorial image denoted by

$$F_{AB\dot{C}\dot{D}} = \tfrac{1}{2}g_{\mu A\dot{C}}F^{\mu\nu}g_{\nu B\dot{D}}\tfrac{1}{2}, \tag{3.8}$$

and therefore,

$$F_{AB\dot{C}\dot{D}} = (\epsilon + p)(u_{A\dot{C}}u_{B\dot{D}} - \tfrac{1}{2}\epsilon_{AB}\epsilon_{\dot{C}\dot{D}}). \tag{3.9}$$

Similarly, the traceless nonlinear electromagnetic field energy-momentum becomes

$$\pi E_{AB\dot{C}\dot{D}} = -H_{P}P_{AB}P_{\dot{C}\dot{D}} = -L_{F}f_{AB}f_{\dot{C}\dot{D}}. \tag{3.10}$$

The image of the traceless Einstein tensor $C^{\mu\nu} := G^{\mu\nu} + \frac{1}{4}g^{\mu\nu}R$ reduces the Einstein equations to the following relations:

$$C_{AB\dot{C}\dot{D}} = 8\pi(F_{AB\dot{C}\dot{D}} + E_{AB\dot{C}\dot{D}}) = 8\pi(\epsilon + p)(u_{A\dot{C}}u_{B\dot{D}} - \tfrac{1}{2}\epsilon_{AB}\epsilon_{\dot{C}\dot{D}}) - 8H_{P}P_{AB}P_{\dot{C}\dot{D}}, \tag{3.11a}$$

$$-\tfrac{1}{4}R = \lambda + 2\pi(3p - \epsilon) + 2(PH_{P} + \check{Q}H_{\check{Q}} - H). \tag{3.11b}$$

Denoting the conventional conformal curvature by the totally symmetric and complex object

$$C_{ABCD} := \tfrac{1}{8}S^{\mu\nu}{}_{AB}C_{\mu\nu\rho\sigma}S^{\rho\sigma}{}_{CD}, \tag{3.12}$$

the Bianchi identifies (2.20) yield

$$\nabla^{D}{}_{D}C_{ABCD} + \nabla_{(A}{}^{\dot{A}}C_{BC)\dot{D}\dot{A}} = 0, \tag{3.13a}$$

$$\nabla^{B\dot{D}}C_{AB\dot{C}\dot{D}} + \tfrac{1}{8}\nabla_{A\dot{C}}R = 0. \tag{3.13b}$$

Particle conservation (2.2b) and velocity normalization take the forms $\nabla^{A\dot{B}}(nu_{A\dot{B}}) = 0$ and $u^{A\dot{B}}u_{A\dot{B}} = 2$.

The original tensors are recovered from the spinorial images by applying the inversion relations originating from the duality properties of the spin tensor and its complex conjugate and the normalization of the Pauli matrices ($\delta^{\mu}{}_{\nu} = -\frac{1}{2}g^{\mu}{}_{A\dot{B}}g_{\nu}{}^{A\dot{B}}$) given by

$$\tfrac{1}{2}S_{\alpha\beta}{}^{AB}S^{\gamma\delta}{}_{AB} = \delta_{\alpha\beta}{}^{\gamma\delta} + (i/\sqrt{-g})\epsilon_{\alpha\beta}{}^{\gamma\delta} \tag{3.14}$$

and its complex conjugate.

We next recall briefly some algebraic properties of the electromagnetic field tensors which are necessary for determining characteristic surfaces. A discussion of greater depth from both the mathematical and physical points of view may be found in Ref. 1 or 20. Considerations of gauge freedom can also be found there. The electromagnetic field tensor $f_{\mu\nu}$ is a real skew symmetric second rank tensor which is called simple if $\check{G} = 0$, null if $F + \check{G} = 0$, and algebraically general if $F + \check{G} \neq 0$. If $f_{\mu\nu}$ is simple, then (and only then) there exist real a_{μ} and b_{ν} such that $f_{\mu\nu} = a_{\mu}b_{\nu} - a_{\nu}b_{\mu}$. The spinorial image $f_{AB} = f_{(AB)}$ always has complex factorization

$$f_{AB} = \alpha_{(A}\beta_{B)}, \tag{3.15}$$

where α_{A}, β_{A} are the principal spinors. Moreover, since $\alpha^{A}\beta_{A}$ and $F + \check{G}$ vanish simultaneously, for the null case

$$f_{AB} = \tfrac{1}{4}fk_{A}k_{B}, \tag{3.16}$$

where the, in general complex, f has dimensions of $f_{\mu\nu}$ and k_{A} is a dimensionless spinor. When $f_{\mu\nu}$ is algebraically general, then (3.15) implies

$$F + \check{G} = 4f_{AB}f^{AB} = -2(\alpha^{A}\beta_{A})^{2} \neq 0. \tag{3.17}$$

Consequently, f_{AB} can always be written as

$$f_{AB} = -\tfrac{1}{2}(\mathscr{E} + i\check{\mathscr{B}})k_{(A}l_{B)}, \tag{3.18}$$

with l_{A} a second dimensionless spinor linearly independent of k_{A} and normalized according to $k^{A}l_{A} = 1$ and $\mathscr{E} \geqslant 0$. Using (3.18) in (3.17)

$$F + \check{G} = -\tfrac{1}{2}(\mathscr{E} + i\check{\mathscr{B}})^{2} \rightarrow \begin{cases} F = \frac{1}{2}(\check{\mathscr{B}}^{2} - \mathscr{E}^{2}) \\ \check{G} = -i\mathscr{E}\check{\mathscr{B}} \end{cases}. \tag{3.19}$$

Here $\check{\mathscr{B}}$ is a pseudoinvariant and without losing generality a coordinate frame can be selected such that $i\check{G} \geqslant 0$, where both $\mathscr{E} \geqslant 0$ and $\check{\mathscr{B}} \geqslant 0$. Inverting yields

$$\mathscr{E} = (|F + \check{G}| - F)^{1/2} \text{ and } \check{\mathscr{B}} = (|F + \check{G}| + F)^{1/2}. \tag{3.20}$$

All these arguments may be repeated for $P_{\mu\nu}$. Assuming an algebraically general $P_{\mu\nu}$ (i.e., $P + \check{Q} \neq 0$), its spinorial image becomes

$$P_{AB} = -\tfrac{1}{2}(\mathscr{S} + i\check{\mathscr{H}})k_{(A}l_{B)}, \tag{3.21}$$

where the non-negative (in an appropriately oriented coordinate system) invariants $\mathscr{S}$ and $\check{\mathscr{H}}$ are

$$\mathscr{S} = (|P + \check{Q}| - P)^{1/2} \text{ and } \check{\mathscr{H}} = (|P + \check{Q}| + P)^{1/2}, \tag{3.22}$$

and there exists an expression equivalent to (3.19) for $P + \check{Q}$.

From (3.6), (3.18), and (3.22),

$$\mathscr{E} + i\check{\mathscr{B}} = (H_P + iH_{\check{Q}})(\mathscr{D} + i\check{\mathscr{H}}) \tag{3.23}$$

and it is natural to pass from $(F,\check{G})$ to $(\mathscr{E},\check{\mathscr{B}})$ and from $(P,\check{Q})$ to $(\mathscr{D},\check{\mathscr{H}})$ as the pairs of independent invariants. Assuming temporarily that the condition for inversions with respect to $\mathscr{D}$ and $\check{\mathscr{H}}$,

$$\partial(\mathscr{E},\check{\mathscr{B}})/\partial(\mathscr{D},\check{\mathscr{H}}) = H^2_{\mathscr{D}\check{\mathscr{H}}} - H_{\mathscr{D}\mathscr{D}}H_{\check{\mathscr{H}}\check{\mathscr{H}}} \neq 0, \tag{3.24}$$

is satisfied, it is not difficult to show simultaneously the implications

$$H_P + H_{\check{Q}} = \frac{-H_{\mathscr{D}} + iH_{\check{\mathscr{H}}}}{\mathscr{D} + i\check{\mathscr{H}}} \leftrightarrow L_F + L_{\check{G}} = \frac{-L_{\mathscr{E}} + iL_{\check{\mathscr{B}}}}{\mathscr{E} + i\check{\mathscr{B}}} \tag{3.25a}$$

and

$$\{\mathscr{E} = -H_{\mathscr{D}}, \check{\mathscr{B}} = H_{\check{\mathscr{H}}}\} \leftrightarrow \{\mathscr{D} = -L_{\mathscr{E}}, \check{\mathscr{H}} = L_{\check{\mathscr{B}}}\}. \tag{3.25b}$$

Also, a direct calculation of the energy density implies that it remains assuredly non-negative if and only if $\mathscr{E}\mathscr{D} + \check{\mathscr{B}}\check{\mathscr{H}} \geqslant 0$; but the equality requires $H_P = 0$, which contradicts the correspondence limit, hence

$$\mathscr{E}\mathscr{D} + \check{\mathscr{B}}\check{\mathscr{H}} > 0, \tag{3.26}$$

which from (3.25) may be equivalently expressed as

$$H_P > 0 \text{ or } L_F > 0. \tag{3.27}$$

Similarly, a positive trace for the energy-momentum tensor

$$\pi E^{\alpha}{}_{\alpha} = \tfrac{1}{2}(-\mathscr{E}\mathscr{D} + \check{\mathscr{B}}\check{\mathscr{H}}) - H \geqslant 0 \tag{3.28}$$

(a requirement of the virial theorem) is equivalent to

$$PH_P + \check{Q}H_{\check{Q}} - H \geqslant 0 \text{ or } L - FL_F\check{G}L_{\check{G}} \geqslant 0. \tag{3.29}$$

We will consistently accept $P_{\mu\nu}$ as the fundamental and $f_{\mu\nu}$ as the secondary object. Consequently, if there are values of $(P,\check{Q})$ which violate the first of either (3.27) or (3.29), they must be rejected as physically inadmissable. These conditions can be interpreted in two ways:(1) as restricting the family of admissible structure functions, (2) as restricting the physically admissible values of $(P,\check{Q})$. Occasionally these conditions hold for every $(P,\check{Q})$ as in the case of the linear theory where $H = P$. When $P_{\mu\nu}$ is null, the correspondence principle implies

$$H_P = 1, H_{\check{Q}} = 0, \text{ and } H_{P\check{Q}} = 0 \tag{3.30}$$

for zero values of the invariants. Therefore,

$$P_{\mu\nu} = f_{\mu\nu} \leftrightarrow P_{AB} = f_{AB} = \tfrac{1}{4} f k_A k_B \tag{3.31}$$

and it follows that the inequality conditions are automatically met. The inequalities (3.27) and (3.29) are important in the further development of the characteristic surface theory.

The dynamic equations of nonlinear electrodynamics presented in Sec. 2 and 3 obtain a most plausible interpretation when the concepts of the electric and magnetic field vectors and the electric and magnetic induction vectors are introduced.[21] The content of these sections then corresponds closely to the Lorentz theory of electrons, where the structure relations

$$D^{\alpha} = \epsilon E^{\alpha} \text{ and}$$
$$\check{B}^{\alpha} = \mu \check{H}^{\alpha} \tag{3.32}$$

are postulated. Due to the properties of the medium ϵ and μ may be different from unity. In our case the circumstances are comparable, but the inductions are more general linear combinations of the intensities,

$$D^{\alpha} = \frac{1}{H_P} E^{\alpha} - i\frac{H_{\check{Q}}}{H_P}\check{H}^{\alpha} \text{ and}$$
$$\check{B}^{\alpha} = \frac{1}{L_F}\check{H}^{\alpha} + i\frac{L_{\check{G}}}{L_F} E^{\alpha}. \tag{3.33}$$

Also, D^{α} can be $\neq E^{\alpha}$, $\check{B}^{\alpha}$ can be $\neq \check{H}^{\alpha}$ due only to the basic nonlinearity (which does not require the presence of any medium). When however, for example, $H_{\check{Q}} = 0$, $L_{\check{G}} = 0$ then $1/H_P$ plays the role of ϵ and $1/L_F$ of μ; or when the field is of null type, then automatically $D^{\alpha} = E^{\alpha}$ and $\check{B}^{\alpha} = \check{H}^{\alpha}$ due to the properties of the structure function. In addition, when the field is algebraically general, there exists a distinguished orientation determined by the energy current for which the relations among the inductions and intensities take the simple form (3.32), where

$$\epsilon = \mathscr{D}/\mathscr{E} = -2\,\partial L/\partial(\mathscr{E}^2) \text{ and}$$
$$\mu = \check{\mathscr{B}}/\check{\mathscr{H}} = 2\,\partial H/\partial(\check{\mathscr{H}}^2). \tag{3.34}$$

Consequently, there is some justification for denoting the ratios ϵ and μ as the electric permittivity and the magnetic permeability. Moreover, in the appropriate limits these equations are formally identical to the conventional equations of electrodynamics in macroscopic media with point-like sources. The complete supporting details of this interpretation of nonlinear electrodynamics are found in Refs. 1 and 20.

4. SMALL PERTURBATIONS AND CHARACTERISTIC SURFACES

In this section, the equations determining the characteristic surfaces for nonlinear electrodynamics in a gravitational field corresponding to the system's set of dynamic equations are developed. The resulting complementary partial differential equations for perturbations of various field gradients are linear with variable coefficients determined by the background fields. Therefore, in principle, they can be solved with standard techniques. The equations are manipulated in spinorial form, because the application of the notation simplifies further algebraic calculation considerably. Our agruments are local (at a fixed point), but have analytic implications. In the theory of small perturbations, the structure equations are considered as central. Conveniently, these particular relations are algebraic, enabling their thorough investigation which eventually results in the theorems on the propagation of discontinuities in the background. The basic problem of characteristic surfaces consists of deriving the necessary conditions, from the perturbed dynamic equations, which permit the existence of nontrivial discontinuities of the first derivatives of the field variables.

A surface $S(x) = \text{const}$ (corresponding to a particular $P_{\mu\nu}$) is said to be characteristic of the object $F(x)$, if the derivatives of its small perturbations of $\delta F_{,\alpha}$ can posses nontrivial discontinuities on S. All quantities denoted by $\delta(\cdots)$ are proportional to some parameter of smallness. The discontin-

uous jump of $F(x)$ at x on the surface S is defined by

$$|[F]|:=\lim_{x_\pm\to x}[F(x_+)-F(x_-)], \tag{4.1}$$

where x_+ and x_- are points located on opposite sides of S along the normal at the point x. The positive side is selected by the direction of the gradient $S_{;\alpha}$. Outside of the surface, the background object F and its first derivatives are continuous in the entire region Ω for which it is defined. The jump in the gradient $F_{;\alpha}$ normal to S is

$$|[\delta F_{;\alpha}]|:=\Delta F S_{;\alpha}. \tag{4.2}$$

Infinitesimally perturbing both conditions at the boundary of Ω and each of the various currents for a particular complete solution gives, by hypothesis, a new solution differing from the original only by small perturbations of all physically relevant variables. Application of this assumption in the usual manner to the dynamic equations provides linear equations for the small perturbations given by

$$\text{Maxwell } \nabla^{S\dot A}\delta P^{B}{}_{S}+\nabla^{B\dot S}\delta P^{\dot A}{}_{\dot S}=4\pi J^{\dot A B}, \tag{4.3a}$$

$$\text{Faraday } \nabla^{S\dot A}\delta f^{B}{}_{S}-\nabla^{B\dot S}\delta f^{\dot A}{}_{\dot S}=0, \tag{4.3b}$$

structure

$$\delta f_{AB}=2H_Z\delta P_{AB}+16(H_{ZZ}P^{CD}\delta P_{CD}+H_{Z\dot Z}P^{\dot C\dot D}\delta P_{\dot C\dot D})P_{AB}, \tag{4.3c}$$

$$\text{Bianchi } \nabla^{D\dot A}\delta C_{ABCD}+\nabla_{(A}{}^{\dot D}\delta C_{BC)\dot D}{}^{\dot A}=0, \tag{4.3d}$$

$$\text{special } \nabla^{A\dot D}\delta C_{AB\dot C\dot D}+\tfrac{1}{8}\nabla_{B\dot C}R=0,$$

Einstein

$$\delta C_{AB\dot C\dot D}=-8H_P\delta(P_{AB}P_{\dot C\dot D})-8\delta H_P P_{AB}P_{\dot C\dot D}+8\pi(\epsilon+p)\delta(u_{AB}u_{\dot C\dot D})+8\pi\delta(\epsilon+p)u_{AB}u_{\dot C\dot D}. \tag{4.3e}$$

Assuming that the perturbative jumps are continuous, but their derivatives are not (e.g., $|[\delta P_{\mu\nu}]|=0$ but $|[\delta P_{\mu\nu;\lambda}]|=\Delta P_{\mu\nu}S_{;\lambda}$), defining the spinor image of the surface gradient by

$$S_{A\dot B}:=g^{\mu}{}_{A\dot B}S_{;\mu}\to S^{A\dot S}S_{B\dot S}=-\delta^{A}{}_{B}S^{;\mu}S_{;\mu}, \tag{4.4}$$

and utilizing the set (4.3), the spinor form of the discontinuity equations on the surface can be written in the basic block:

$$\text{from Maxwell } S^{S\dot A}\Delta P^{B}{}_{S}+S^{B\dot S}\Delta P^{\dot A}{}_{\dot S}=0, \tag{4.5a}$$

$$\text{from Faraday } S^{S\dot A}\Delta f^{B}{}_{S}-S^{B\dot S}\Delta f^{\dot A}{}_{\dot S}=0, \tag{4.5b}$$

$$\text{from structure } \Delta f_{AB}=2H_Z\Delta P_{AB}+16P_{AB}(H_{ZZ}P^{CD}\Delta P_{CD}+H_{Z\dot Z}P^{\dot C\dot D}\Delta P_{\dot C\dot D}), \tag{4.5c}$$

$$\text{from Bianchi } S^{D\dot A}\Delta C_{ABCD}+S_{(A}{}^{\dot D}\Delta C_{BC)\dot D}{}^{\dot A}=0, \tag{4.5d}$$

$$\text{special } S^{A\dot D}\Delta C_{AB\dot C\dot D}+\tfrac{1}{8}S_{B\dot C}\Delta R=0,$$

from Einstein

$$\Delta C_{AB\dot C\dot D}=-8H_P\Delta(P_{AB}P_{\dot C\dot D}-8\Delta H_P P_{AB}P_{\dot C\dot D}-\tfrac{1}{8}\Delta R=\Delta(H_Z Z+H_{\dot Z}\dot Z-H). \tag{4.5e}$$

The remainder of this work is effectively devoted to the evaluation of the properties of the solutions of these relations for the discontinuities in the derivatives of the various field variables on the characteristic surfaces. Specifically, the necessary conditions permitting the existence of $\Delta P_{AB}\neq 0$ are derived for background fields which are null ($P_{\mu\nu}\neq 0, P+\check Q=0$) and algebraically general ($P+\check Q\neq 0$). The case of a trivial background field ($P_{\mu\nu}=0$) is omitted, since for weak fields the theory coincides identically with the linear electrodynamic case by construction. It must be underlined that we assume $\Delta P_{AB}\neq 0$, but whether Δf_{AB}, etc., vanish or not remains questionable. The possible characteristic surfaces are repeatedly divided into two classes: (1) the null characteristic surfaces (NCS), where $S_{;\mu}S^{;\mu}=0$ and (2) the general characteristic surfaces (GCS), where $S_{;\mu}S^{;\mu}\neq 0$. The symbol Σ is used to denote the product $S_{;\mu}S^{;\mu}$.

5. CHARACTERISTIC SURFACES OF LINEAR ELECTRODYNAMICS WITH GRAVITATION

Reducing the basic characteristic surface equations (4.5) for $P_{\mu\nu}=f_{\mu\nu}$, which corresponds to the linear electrodynamic case, Eqs. (3.30) are encountered with H_{ZZ} and $H_{Z\dot Z}$ real and in general nonvanishing. Moreover, $C_{AB\dot C\dot D}=-8f_{AB}f_{\dot C\dot D}$ with $R=0$. The subcases Δf_{AB} zero or nonzero are evaluated separately.

A. $\Delta f_{AB}\neq 0$ on the characteristic surface

Substituting $P_{AB}=f_{AB}$ into (4.5a,b) and noting (4.4), one has necessarily

$$\det S^{A\dot B}=\tfrac{1}{2}S^{A\dot B}S_{A\dot B}=0\leftrightarrow\Sigma:=S^{;\mu}S_{;\mu}=0\to S_{A\dot B}=S_A S_{\dot B}, \tag{5.1}$$

where S_A is a specific spinor which is not difficult to calculate. Select $\{S_A,\tilde S_A\}$ with $S^A\tilde S_A=1$ as a spinor basis for decomposing Δf_{AB} such that

$$\Delta f_{AB}=:\Delta f\, S_A S_B+\Delta f_1\tilde S_A\tilde S_B+\Delta f_2 S_{(A}\tilde S_{B)}. \tag{5.2}$$

Contracting this with S^B account for (4.5a,b) $\Delta f_1=0=\Delta f_2$; thus for Δf a complex function,

$$\Delta f_{AB}=\Delta f S_A S_B. \tag{5.3}$$

Substituting $C_{AB\dot C\dot D}$ from the introductory paragraph above and (5.1) into the Bianchi identity (4.5d) yields

$$S^{D}\Delta C_{ABCD}+8\Delta f(f_{A\dot B}S^{A}\tilde S^{\dot B})S_A S_B S_C=0. \tag{5.4}$$

For jumps in the totally symmetric conformal curvature, the most general form is

$$\Delta C_{ABCD}=:\Delta C_1 S_A S_B S_C S_D+4\Delta C_2 S_{(A}S_B S_C\tilde S_{D)}+6\Delta C_3 S_{(A}S_B\tilde S_C\tilde S_{D)}+4\Delta C_4 S_{(A}\tilde S_B\tilde S_C\tilde S_{D)}+\Delta C_5\tilde S_A\tilde S_B\tilde S_C\tilde S_D. \tag{5.5}$$

Comparing (5.5), therefore, $\Delta C_1\in\mathbb{C}$ and arbitrary,

$$\Delta C_2=8\Delta f(f_{A\dot B}S^{A}\tilde S^{\dot B}),\ \Delta C_3=\Delta C_4=\Delta C_5=0. \tag{5.6}$$

When f_{AB} is either algebraically general or null but of the form $f_{AB}=\frac{1}{4}f'(S_A-\tilde S_A)(S_B-\tilde S_B)$, since $\Delta C_2\neq 0$, the result is

$$\Delta C_{ABCD}=S_{(A}S_B S_C(\Delta C_1 S_{D)}+8f'\Delta f\tilde S_{D)}), \tag{5.7}$$

which is of type III:[3-1]. If and only if f_{AB} is null and such that $f_{AB}S^{A}\tilde S^{B}=0$, then $S_{;\mu}$ is an eigenvector of the background null field. When this circumstance occurs ΔC_2 vanishes directly and ΔC_{ABCD} is given by the first term of (5.7), which is of type N:[4].

B. $\Delta f_{AB} = 0$ on the characteristic surface

The jump relation from the first Bianchi identity (4.5d) for this subcase requires

$$S^{D\dot{A}}\Delta C_{ABCD} = 0 \rightarrow \begin{cases} \Delta C_{ABCD} = 0 & \text{if } \Sigma \neq 0 \\ \Delta C_{ABCD} \text{ is of type N:[4]} & \text{if } \Sigma = 0. \end{cases} \tag{5.8}$$

Summarizing this straightforward special case, the characteristic surfaces of linear electrodynamics are necessarily null ($\Sigma = 0$) if there exists a nontrivial jump. Specifically, the discontinuities in the derivatives of small perturbations in both the electrodynamic and gravitational fields propagate at "the speed of light," and the only discontinuous jumps in the perturbations of conformal curvature permitted are of the types III:[3-1] and N:[4].

6. CHARACTERISTIC SURFACES OF NONLINEAR ELECTRODYNAMICS WITH GRAVITATION

Regarding P_{AB} as the fundamental object providing a nonlinear electrodynamic solution completing the Einstein equations,

$$C_{AB\dot{C}\dot{D}} = -8H_P P_{AB} P_{\dot{C}\dot{D}}, \tag{6.1a}$$

$$-\tfrac{1}{4}R = \lambda + 2(ZH_Z + \dot{Z}H_{\dot{Z}} - H), \tag{6.1b}$$

and selecting ΔP_{AB} as the generator of the remaining discontinuities, the set of equations (4.5) describe the physical system. Introduce the notation

$$\Delta Z := 8P^{AB}\Delta P_{AB} \tag{6.2}$$

and the traceless energy–momentum tensor of linear electrodynamics,

$$\begin{aligned} \tau^{\mu\nu}[P] &:= -P^{\mu\lambda}P^{\nu}{}_{\lambda} + \tfrac{1}{4}g^{\mu\nu}P^{\rho\sigma}P_{\rho\sigma} \\ &= 4P_{A\dot{B}}P_{CD}S^{\dot{A}C}S^{\dot{B}D}. \end{aligned} \tag{6.3}$$

Then after recognizing that

$$S_A{}^{\dot{A}}S^A{}_{\dot{B}} = (S_{;\mu}S^{;\mu})\delta^{\dot{A}}{}_{\dot{B}} =: \Sigma\delta^{\dot{A}}{}_{\dot{B}}, \tag{6.4}$$

and after substituting (4.5c) into (4.5b) using (4.5a), you deduce that successively multiplying by $S_A{}^{\dot{A}}$ and $-2P^{\dot{A}}{}_{\dot{B}}$ gives

$$\begin{aligned} &[(\tfrac{1}{2}H_P + \dot{Z}H_{\dot{Z}\dot{Z}})\Sigma + H_{Z\dot{Z}}\tau^{\mu\nu}S_{;\mu}S_{;\nu}]\Delta\dot{Z} \\ &\quad + [\dot{Z}H_{Z\dot{Z}}\Sigma + H_{ZZ}\tau^{\mu\nu}S_{;\mu}S_{;\nu}]\Delta Z = 0. \end{aligned} \tag{6.5}$$

This expression and its complex conjugate form a system of linear homogeneous equations for ΔZ and $\Delta\dot{Z}$, whose determinant is

$$\begin{aligned} \Delta &:= |(\tfrac{1}{2}H_P + \dot{Z}H_{\dot{Z}\dot{Z}})\Sigma + H_{Z\dot{Z}}\tau^{\mu\nu}S_{;\mu}S_{;\nu}|^2 \\ &\quad - |\dot{Z}H_{Z\dot{Z}}\Sigma + H_{ZZ}\tau^{\mu\nu}S_{;\mu}S_{;\nu}|^2, \end{aligned} \tag{6.6}$$

which must vanish whenever $\Delta Z \neq 0$ as a direct algebraic consequence of the discontinuity relations. In general, we claim

$$\Delta P_{AB} \neq 0 \rightarrow \Delta = 0. \tag{6.7}$$

This implication is conveniently proved by contradiction; hence assume that simultaneously $\Delta P_{AB} \neq 0$ and $\Delta \neq 0$. From (6.5), $\Delta Z = 0$ and then $H_P\Sigma\Delta P_{A\dot{B}} = 0$, or for $H_P > 0$ we infer a NCS with $S_{A\dot{B}}S^{A\dot{B}} = 0$. $S_{A\dot{B}}$ has the algebraic form $S_{A\dot{B}} = S_A\bar{S}_{\dot{B}}$ which, when introduced into (4.5a and b), yields the expressions

$$\Delta P_{AB}S^B = i\Delta P S_A \text{ and } \Delta f_{AB}S^B = \Delta f S_A, \tag{6.8}$$

where ΔP and Δf are both real numbers. Using the reduced form of the structure relation (4.5c) in the second of these equations necessitates

$$\Delta f = 2iH_Z\Delta P \rightarrow \Delta P = 0 = \Delta f, \tag{6.9}$$

because the real part of $2H_Z$ is $H_P > 0$ by hypothesis. Consequently, there exist nonvanishing complexes $\Delta P'$ and $\Delta f'$ such that

$$\begin{aligned} &\Delta P_{AB} = \Delta P'\, S_{(A}S_{B)} \text{ and } \Delta f_{AB} = \Delta f' S_{(A}S_{B)} \text{ with} \\ &\Delta f' = 2H_Z\Delta P', \end{aligned} \tag{6.10}$$

which due to $\Delta Z = 8P^{AB}\Delta P_{AB} = 0$, implies

$$P_{AB}S^AS^B = 0. \tag{6.11}$$

Independent of whether the background is trivial ($P_{AB} = 0$) or nontrivial ($P_{AB} = P_{(A}S_{B)} \neq 0$), we encounter

$$\Sigma = 0 \text{ and } \tau^{\mu\nu}S_{;\mu}S_{;\nu} = 0, \tag{6.12}$$

requiring that $\Delta = 0$, a contradiction. Thus the implication has been established. It remains to demonstrate the existence of nontrivial ΔP_{AB} (and Δf_{AB}) when $\Delta = 0$, which will be done by explicit calculation in what follows.

A. The class of NCS ($\Sigma = 0$)

Proceeding as in the proof above, Eqs. (4.5a)–(4.5c) lead to (6.8) with

$$\Delta f = 2iH_Z\Delta P - 2\Delta H_Z P^{AB}S_A\tilde{S}_B,\ \tilde{S}_AS^A = 1, \tag{6.13}$$

where

$$\begin{aligned} \Delta H_Z &:= H_{ZZ}\Delta Z + H_{Z\dot{Z}}\Delta\dot{Z} \\ &= 8(H_{ZZ}P^{AB}\Delta P_{AB} + H_{Z\dot{Z}}P^{A\dot{B}}\Delta P_{A\dot{B}}). \end{aligned} \tag{6.14}$$

The determinant reduces to

$$\begin{aligned} \Delta &= |H_{Z\dot{Z}}{}^2 - H_{ZZ}H_{\dot{Z}\dot{Z}}|\cdot|\tau^{\mu\nu}S_{;\mu}S_{;\nu}|^2 \\ &= |H_{P\check{Q}}{}^2 - H_{PP}H_{\check{Q}\check{Q}}|\cdot|2P^{AB}S_AS_B|^4 = 0. \end{aligned} \tag{6.15}$$

1. Equation (6.15) and $H_{P\check{Q}}{}^2 - H_{PP}H_{\check{Q}\check{Q}} = 0 \rightarrow P_{AB}S^AS^B \neq 0$

This can hold locally for specific values of P and $\check{Q}$ or globally for all admissible values, from the structure of H. Consider $F := F(H_P, H_{\check{Q}})$ whose differential is given by $(H_{PP}F_{,H_P} + H_{P\check{Q}}F_{,H_{\check{Q}}})dP + (H_{P\check{Q}}F_{,H_P} + H_{\check{Q}\check{Q}}F_{,H_{\check{Q}}})d\check{Q}$. Observe that it is possible to encounter a nontrivial F with vanishing differential, because the linear homogeneous system of equations

$$H_{PP}F_{,H_P} + H_{P\check{Q}}F_{,H_{\check{Q}}} = 0, \quad H_{P\check{Q}}F_{,H_P} + H_{\check{Q}\check{Q}}F_{,H_{\check{Q}}} = 0 \tag{6.16}$$

has vanishing determinant. This subcase may globally yield the existence of a $F(H_P, H_{\check{Q}}) = \text{const}$, which constrains the possible structure functions. The linear theory ($H = P$) is an important, and trivial, subclass belonging to the case discussed.

Satisfying (6.13) with $\Delta H_Z = 0$ implies in a manner identical to the proof of (6.7) that $\Delta P = 0 = \Delta f$, leading again to (6.10). When $P_{AB}S^AS^B \neq 0$ also $H_{Z\dot{Z}}{}^2 - H_{ZZ}H_{\dot{Z}\dot{Z}} = 0$ if there exists a nontrivial solution, suggesting a further separation into two subcases. If ΔH_Z of

(6.14) vanishes due to $H_{ZZ} = H_{Z\dot{Z}} = 0$, then $\Delta P'$ remains arbitrary and ΔP_{AB} contains two arbitrary constants. Or, for the alternative subcase, if $|H_{ZZ}| = |H_{Z\dot{Z}}| \neq 0$, you encounter

$$\frac{\Delta P'}{\Delta \dot{P}'} = -\frac{H_{Z\dot{Z}}}{H_{ZZ}} \frac{P_{A\dot{B}} S^{A} S^{\dot{B}}}{P_{AB} S^{A} S^{B}}, \tag{6.17}$$

indicating the phase of the jump $\Delta P'$ is determined when the structure function and field are known. Only $|\Delta P'|$ remains arbitrary and ΔP_{AB} depends on one arbitrary constant.

Substituting the jump expression from the Einstein equations (4.5e) into that of the first Bianchi identity (4.5d) and again using the content of (6.10), you obtain

$$\Delta C_{ABCD} = S_{(A} S_B S_C (\Delta C_1 S_{D)} - 32 H_P \Delta P' P_{A\dot{B}} S^{\dot{A}} \tilde{S}^{\dot{B}} \tilde{S}_{D)}), \tag{6.18}$$

where ΔC_1 is complex and arbitrary. Consequently, the jump in conformal curvature on the characteristic surface is of type III:[3-1], except when the background nonlinear electrodynamic field is null where the gradient $S_{;\mu}$ is the same vector resultant from a jump of type N:[4].

2. Equation (6.15) and $H_{P\check{\mathscr{D}}}{}^2 - H_{PP} H_{\check{\mathscr{D}}\check{\mathscr{D}}} \neq 0 \rightarrow P_{AB} S^A S^B = 0 \rightarrow P_{AB} = P_{(A} S_{B)}$.

When the background is trivial the implication is automatically fulfilled; but if $P_{AB} \neq 0$, $S_{;\mu}$ is an eigenvector of $P_{\mu\nu}$, i.e., the relation above may be translated to the equivalent tensorial image

$$P_{\mu}{}^{\rho} S_{;\rho} = \lambda S_{;\mu} \rightarrow \tau^{\mu\nu} S_{;\mu} S_{;\nu} = 0, \tag{6.19}$$

where for algebraically general $P_{AB} = \frac{1}{2}(\mathscr{D} + i\check{\mathscr{H}}) k_{(A} l_{B)}$, $k^A l_A = 1 \rightarrow$ there exists real nonvanishing $\lambda = \mp \frac{1}{4}\mathscr{D}$, depending upon whether $S_{;\mu} = k_\mu$ or l_μ, and where for null $P_{AB} = \frac{1}{4} P k_A k_B \rightarrow \lambda = 0$ with $\epsilon^{\mu\nu\lambda\rho} k_{\mu;\nu} k_{\lambda;\rho} = 0$.

Satisfying (6.13) when $\Delta H_Z \neq 0$, one concludes immediately from the structure relation (4.5c) that

$$\Delta f_{(A} S_{B)} = 2 H_Z \Delta P_{(A} S_{B)} + 2 P_{AB} \Delta H_Z. \tag{6.20}$$

The background field acquires the form $P_{AB} = P_{(A} S_{B)}$, where (6.19) holds with

$$\Delta f = 2i \Delta P H_Z - \Delta H_Z P^A S_A \tag{6.21}$$

and

$$\Delta H_Z = 8i \Delta P (H_{ZZ} P^A S_A - H_{Z\dot{Z}} P^{\dot{A}} S_{\dot{A}}) \neq 0, \tag{6.22}$$

which implies $\Delta P \neq 0$. Hence the structure function must be nonlinear so that at least one of H_{ZZ} or $H_{Z\dot{Z}}$ is different from zero; and the complex invariant of the field $Z = 4 P^{AB} P_{AB} = -2 (P^A S_A)^2 \neq 0$, hence the field is algebraically general. Transforming to the invariants $\mathscr{D}$ and $\check{\mathscr{H}}$ defined by $Z := P + \check{Q} = -\frac{1}{2}(\mathscr{D} + i\check{\mathscr{H}})^2$ and noting that, since Δf and $\Delta P \neq 0$ are real, the structure function is constrained by the condition $H_{\check{\mathscr{H}}\check{\mathscr{H}}} = 0$, we have

$$2\Delta f = -\Delta P H_{\mathscr{D}\check{\mathscr{H}}}. \tag{6.23}$$

Also

$$\Delta P_{AB} S^B = \Delta P' S_A + i \Delta P \tilde{S}_A \text{ and } \Delta f_{AB} S^B = \Delta f' S_A + \Delta f \tilde{S}_A, \tag{6.24}$$

with $\Delta f' = 2 H_z \Delta P'$, where $\Delta f'$ and $\Delta P'$ are in general complex. Therefore, the general forms for the jumps are

$$\Delta P_{AB} = 2 \Delta P' S_A S_B + 2i \Delta P \tilde{S}_{(A} S_{B)}, \tag{6.25a}$$

$$\Delta f_{AB} = 2 \Delta f' S_A S_B + 2 \Delta f \tilde{S}_{(A} S_{B)}. \tag{6.25b}$$

Here ΔP_{AB} depends on three arbitrary constants due to the complex $\Delta P'$ and the real ΔP. The background field is given by

$$P_{AB} = \mp \tfrac{1}{2}(\mathscr{D} + i\check{\mathscr{H}}) \tilde{S}_{(A} S_{B)}. \tag{6.26}$$

The determinant condition ($\mathbf{\Delta} = 0$) is automatically satisfied and

$$\Delta H_Z = (i \Delta P / 4 P^A S_A)[H_P - i(H_{\mathscr{D}\check{\mathscr{H}}} + i H_{\check{Q}})]. \tag{6.27}$$

Regarding the relevance of these last electrodynamic jumps, observe that the constraint $H_{\check{\mathscr{H}}\check{\mathscr{H}}} = 0$ contradicts the correspondence assumption $H \cong \frac{1}{2}(\check{\mathscr{H}}^2 - \mathscr{D}^2)$ for small values of $\mathscr{D}$ and $\check{\mathscr{H}}$. Therefore, probably the only cases of physical interest are those possessing constant valued invariants for some set of points. From (6.25), $\Delta P_{\mu\nu}$ cannot be a null bivector; yet if additionally $H_{\mathscr{D}\check{\mathscr{H}}} = 0$, then $\Delta f = 0$ and $\Delta f_{\mu\nu}$ is a null bivector (or even trivial if $\Delta P' = 0 \rightarrow \Delta f' = 0$). If this pathologic situation occurs, then $\mathscr{L}(\check{\mathscr{E}}, \check{\mathscr{B}})$ does not exist for the corresponding values of $\mathscr{D}$ and $\check{\mathscr{H}}$.

Examining the first Bianchi identity (4.5d) for this subcase and multiplying independently by $\tilde{S}^{\dot{A}}$ and $S^{\dot{A}}$ gives

$$S^D \Delta C_{ABCD} = 4 H_P [(\mathscr{D} - i\check{\mathscr{H}}) \Delta P' S_A S_B S_C + 2i \mathscr{D} \Delta P S_{(A} S_B \tilde{S}_{C)}] \tag{6.28}$$

and

$$|Z|(\Delta H_Z + \Delta H_{\dot{Z}}) = 0 \rightarrow \mathrm{Re} \Delta H_Z = 0. \tag{6.29}$$

But

$$\Delta H_Z = 4i \Delta P [(\mathscr{D} + i\check{\mathscr{H}}) H_{ZZ} - (\mathscr{D} - i\check{\mathscr{H}}) H_{Z\dot{Z}}]; \tag{6.30}$$

hence, setting the real part to zero places an additional restriction on the structure function,

$$\check{\mathscr{H}} H_P + \mathscr{D}(H_{\mathscr{D}\check{\mathscr{H}}} + i H_{\check{Q}}) = 0. \tag{6.31}$$

The most general form of the curvature jump becomes

$$C_{ABCD} + S_{(A} S_B (\Delta C_1 S_C + a \tilde{S}_C)(S_{D)} + b \tilde{S}_{D)}), \tag{6.32}$$

where $a + b \Delta C_1 = 16 H_P (\mathscr{D} - i\check{\mathscr{H}}) \Delta P'$ and $a \cdot b = 16 i H_P \mathscr{D} \Delta P$. That is, ΔC_{ABCD} is to type D:[2-1-1] in this subcase.

B. The class of GCS ($\Sigma \neq 0$)

Multiplying by $S_A{}^{\dot{A}}$ the result of substituting (4.5c) into (4.5b) and using (4.5a) gives

$$H_P \Sigma \Delta P^{\dot{B}}{}_{\dot{A}} + (H_{Z\dot{Z}} \Delta Z + H_{\dot{Z}\dot{Z}} \Delta \dot{Z}) \Sigma P^{\dot{B}}{}_{\dot{A}} - (H_{ZZ} \Delta Z + H_{Z\dot{Z}} \Delta \dot{Z}) S_{A\dot{A}} S^{B\dot{B}} P^A{}_B = 0. \tag{6.33}$$

Under the basic assumption of the class, solving this for the electrodynamic jump ΔP_{AB} yields

$$\Delta P_{AB} = \Sigma P_{AB} \Delta w + S_A{}^{\dot{A}} S_B{}^{\dot{B}} P_{\dot{A}\dot{B}} \Delta \dot{w}, \tag{6.34}$$

where

$$\Delta w = -(H_{ZZ}\Delta Z + H_{Z\dot{Z}}\Delta\dot{Z})(H_P\Sigma)^{-1}. \tag{6.35}$$

Substituting (6.34) into (6.2) and the result into (6.35), we obtain

$$\rho\Delta w + \sigma\Delta\dot{w} = 0, \tag{6.36}$$

where

$$\rho := (H_P + 2ZH_{ZZ})\Sigma + 2H_{Z\dot{Z}}\tau^{\mu\nu}S_{;\mu}S_{;\nu},$$
$$\sigma := 2\dot{Z}H_{Z\dot{Z}}\Sigma + 2H_{ZZ}\tau^{\mu\nu}S_{;\mu}S_{;\nu}. \tag{6.37}$$

Equation (6.36) and its complex conjugate form a linear homogeneous set of equations whose determinant is precisely Δ. When $\Delta w \neq 0$, necessarily

$$\Delta = |\rho|^2 - |\sigma|^2 = 0, \tag{6.38}$$

which coincides with (6.6). Since $\Delta P_{AB} \neq 0$, GCS can exist only when (1) the background field is nontrivial ($P_{AB} \neq 0$, (2) the jump $\Delta w \neq 0$ (which occurs only when $\Delta Z \neq 0$), and (3) the situation is genuinely nonlinear (at least one of H_{ZZ} or $H_{Z\dot{Z}}$ must be nonzero). We acknowledge that from the structure of (6.34), $\Delta P^{\mu}{}_{\nu}S^{;\nu} = 0$. The same was true for NCS.

Before proceeding with the consideration of null and algebraically general background fields, it is profitable to analyze some algebraic consequences of the Bianchi identities. Multiplying both Bianchi identities (4.5d) by $S^{\dot{A}}{}_{D}$ and taking the symmetric and antisymmetric parts result in

$$\Sigma\Delta C_{ABCD} = S_{(A}{}^{\dot{A}}S_{B}{}^{\dot{B}}\Delta C_{CD)\dot{A}\dot{B}}, \tag{6.39a}$$
$$S_{(A}{}^{\dot{A}}\Delta C_{B)C\dot{A}\dot{B}}S^{C\dot{B}} = 0, \tag{6.39b}$$
$$S^{A\dot{A}}S^{B\dot{B}}\Delta C_{AB\dot{A}\dot{B}} + \tfrac{1}{4}\Delta R\Sigma = 0. \tag{6.39c}$$

For GCS, using the expression for ΔP_{AB} (6.34) and the Einstein equation (6.1),

$$\Delta C_{AB\dot{C}\dot{D}} = -8H_P(S_A{}^{\dot{A}}S_B{}^{\dot{B}}P_{\dot{A}\dot{B}}P_{\dot{C}\dot{D}}\Delta\dot{w} + S_C{}^{\dot{C}}S_{\dot{D}}{}^{\dot{D}}P_{AB}P_{CD}\Delta w, \tag{6.40a}$$
$$-\tfrac{1}{8}\Delta R = \Delta(H_P P + H_{\breve{Q}}\breve{Q} - H) = \Delta H_Z + \Delta H_{\dot{Z}}. \tag{6.40b}$$

Using $\Delta H_Z = -H_P\Sigma\Delta w$, $\Delta H_P = -H_P(\Delta w + \Delta\dot{w})\Sigma$, and $\Delta H_{\breve{Q}} = -H_{\breve{Q}}(\Delta w - \Delta\dot{w})\Sigma$, these imply

$$S^{B\dot{D}}\Delta C_{AB\dot{C}\dot{D}} = -H_P\Sigma(Z\Delta w + \dot{Z}\Delta\dot{w})S_{A\dot{C}}, \tag{6.41a}$$
$$\tfrac{1}{8}\Delta R = H_P\Sigma(Z\Delta w + \dot{Z}\Delta\dot{w}). \tag{6.41b}$$

Substituting (6.40a) into (6.39a) provides

$$\Sigma\Delta C_{ABCD} = -8H_P(\Sigma^2\Delta w P_{(AB}P_{CD)} + \Delta\dot{w}S_{(A}{}^{\dot{A}}S_B{}^{\dot{B}}S_C{}^{\dot{C}}S_{D)}{}^{\dot{D}}P_{\dot{A}\dot{B}}P_{\dot{C}\dot{D}}). \tag{6.42}$$

1. Null background electrodynamic field ($P_{AB} = \tfrac{1}{4}Pk_Ak_B$)

$P \neq 0$ is in general complex. Due to correspondence for the partial evaluated at $Z = 0$; $H_P = 1$, $H_{\breve{Q}} = H_{P\breve{Q}} = 0$ such that $4H_{ZZ} = H_{PP} + H_{\breve{Q}\breve{Q}}$, $4H_{Z\dot{Z}} = H_{PP} - H_{\breve{Q}\breve{Q}}$. The expressions for ρ and σ become

$$\rho = \Sigma + \tfrac{1}{2}(H_{PP} - H_{\breve{Q}\breve{Q}})\tau^{\mu\nu}S_{;\mu}S_{;\nu},$$
$$\sigma = \tfrac{1}{2}(H_{PP} + H_{\breve{Q}\breve{Q}})\tau^{\mu\nu}S_{;\mu}S_{;\nu}, \tag{6.43}$$

and

$$\Delta = \rho^2 - \sigma^2 = (\rho + \sigma)(\rho - \sigma) = 0. \tag{6.44}$$

There exist two alternatives, either characteristic type

$$P\text{: } \rho + \sigma = \Sigma + H_{PP}\tau^{\mu\nu}S_{;\mu}S_{;\nu} = 0 \text{ or}$$
$$\breve{Q}\text{: } \rho - \sigma = \Sigma - H_{\breve{Q}\breve{Q}}\tau^{\mu\nu}S_{;\mu}S_{;\nu} = 0, \tag{6.45}$$

with $\tau^{\mu\nu}S_{;\mu}S_{;\nu} \neq 0$.

When $Z = 0$, in the exceptional case where

$$H_{PP} + H_{\breve{Q}\breve{Q}} = 0 \quad \text{with} \quad \rho = 0 = \sigma, \tag{6.46}$$

the two characteristics coincide and there exists a single characteristic equation

$$\Sigma = H_{\breve{Q}\breve{Q}}\tau^{\mu\nu}S_{;\mu}S_{;\nu} \neq 0, \tag{6.47}$$

where the inequality is valid when the single surface is GCS. Equation (6.36) is automatically satisfied with arbitrary complex $\Delta w \neq 0$, and hence the solution for ΔP_{AB} (6.34) contains two real arbitrary constants. Calculating the product $4\Delta P_{AB}\Delta P^{AB}$ demonstrates that $\Delta P_{\mu\nu}$ is algebraically general, although it is a simple bivector. If $S_{;\mu} \to \lambda k_{\mu}$, then the GCS limits to a NCS, the characteristic equation remains fulfilled, and $\Delta P_{\mu\nu}$ becomes a null bivector.

In the general case where

$$H_{PP} + H_{\breve{Q}\breve{Q}} \neq 0 \tag{6.48}$$

the characteristic surfaces are distinct, and one finds

$$P\text{: } \rho = -\sigma = -\tfrac{1}{2}(H_{PP} + H_{\breve{Q}\breve{Q}})\tau^{\mu\nu}S_{;\mu}S_{;\nu} \neq 0,$$
$$\breve{Q}\text{: } \rho = \sigma = \tfrac{1}{2}(H_{PP} + H_{\breve{Q}\breve{Q}})\tau^{\mu\nu}S_{;\mu}S_{;\nu} \neq 0 \tag{6.49}$$

when the surfaces are GCS. Correspondingly, condition

(6.36) reads, respectively,

$$P\text{: } \Delta w + \Delta\dot{w} = 0 \quad \text{and} \quad \breve{Q}\text{: } \Delta w - \Delta\dot{w} = 0. \tag{6.50}$$

Thus, Δw is either purely real or imaginary, and ΔP_{AB} contains only one arbitrary real (multiplicative) constant. $\Delta P_{\mu\nu}$ is algebraically general in both cases. Notice, it may be that one surface is a NCS, as in the situation where $H = H(P) \to H_{\breve{Q}\breve{Q}} = 0$; then the above argument applies only to the one GCS.

In a normalized spinor base $\{k_A, l_A\}$ such that $k^A l_A = 1$, $S_{A\dot{B}}$ may be expanded in the form

$$S_{A\dot{B}} = xk_A k_{\dot{B}} + yl_A l_{\dot{B}} + zk_A l_{\dot{B}} + \dot{z} l_A k_{\dot{B}} \tag{6.51}$$

with x,y real and z complex, giving

$$-\Sigma = \tfrac{1}{2} S^{A\dot{B}} S_{A\dot{B}} = xy - z\dot{z} \neq 0$$

and

$$-\tau^{\mu\nu} S_{;\mu} S_{;\nu} = \tfrac{1}{4} |P|^2 (xy + z\dot{z}) \neq 0. \tag{6.52}$$

Respecting the constraints on the null background field dictated by correspondence and defining

$$\eta^A := \eta_1 k^A + \eta_2 l^A \tag{6.53}$$

with $\eta^A S_A{}^A k_{\dot{A}} = -(\eta_1 y - \eta_2 z)$, (6.42) has the form

$$\begin{aligned}\Sigma\Delta C_{ABCD} = & -\tfrac{1}{2}[(xy - z\dot{z})^2 P^2 \Delta w k_A k_B k_C k_D \\ & + \dot{P}^2 \Delta\dot{w}(yk_{(A} + zl_{(A})(yk_B + zl_B) \\ & \times (yk_C + zl_C)(yk_{D)} zl_{D)})].\end{aligned} \tag{6.54}$$

Therefore,

$$\begin{aligned}\Sigma\Delta C_{ABCD}\eta^A\eta^B\eta^C\eta^D \\ = -\tfrac{1}{2}[\Delta w P^2 (xy - z\dot{z})^2 \eta_2^4 + \Delta\dot{w}\dot{P}^2(-y\eta_2 + z\eta_1)^4]\end{aligned} \tag{6.55}$$

which, when $z \neq 0$, has the characteristic polynomial

$$\left[\eta - \frac{y}{z}\right]^4 + \left[\frac{x}{z}\frac{y}{z} - \frac{\dot{z}}{z}\right]^2 \frac{\Delta w P^2}{\Delta\dot{w}\dot{P}^2} = 0, \tag{6.56}$$

whose distinct roots are

$$\eta_n = \frac{y}{z} + \left\{\frac{\Delta w P^2}{\Delta\dot{w}\dot{P}^2}\right\}^{1/4}\left\{\frac{x}{z}\frac{y}{z} - \frac{\dot{z}}{z}\right\}^{1/2} e^{in\pi/2}, \quad n = 0,1,2,3 \tag{6.57}$$

resulting in a ΔC_{ABCD} of the type I:[1-1-1-1]. Where $z = 0$, (6.55) implies $\eta_2 = 0$ and there exists a quadruple degenerate root, yielding a conformal curvature jump of type N:[4]. These jumps occur for characteristics of both types.

2. Algebraically general background field ($P_{AB} = -\frac{1}{2}(\mathscr{D} + i\breve{\mathscr{H}})k_{(A}l_{B)}$)

For this subclass where $S_{A\dot{B}}$ has the form (6.51), the invariants are conveniently written as functions of the parameters x, y, and z:

$$-\Sigma = xy - z\dot{z} \quad \text{and} \quad -\tau^{\mu\nu} S_{;\mu} S_{;\nu} = |Z|(xy + z\dot{z}), \tag{6.58}$$

where $Z = -\frac{1}{2}(\mathscr{D} + i\breve{\mathscr{H}})^2$ is the complex invariant of the nonlinear electrodynamic field. Introducing these in (6.37) and changing variables one encounters

$$2\rho = -[H_P + H_{\breve{\mathscr{H}}\breve{\mathscr{H}}} + i(H_{\mathscr{D}\breve{\mathscr{H}}} + iH_{\breve{Q}})]xy - [H_P - H_{\mathscr{D}\mathscr{D}} + i(H_{\mathscr{D}\breve{\mathscr{H}}} + iH_{\breve{Q}})]z\dot{z},$$

$$2\sigma = -(\mathscr{D} - i\breve{\mathscr{H}})(\mathscr{D} + i\breve{\mathscr{H}})^{-1}\{[H_P - H_{\breve{\mathscr{H}}\breve{\mathscr{H}}} - i(H_{\mathscr{D}\breve{\mathscr{H}}} + iH_{\breve{Q}})]xy + [H_P + H_{\mathscr{D}\mathscr{D}} - i(H_{\mathscr{D}\breve{\mathscr{H}}} + iH_{\breve{Q}})]z\dot{z}\}, \tag{6.59}$$

which give for (6.38)

$$\Delta = (H_P xy + H_{\mathscr{D}\mathscr{D}} z\dot{z})(H_{\breve{H}\breve{H}} xy - H_P z\dot{z}) - (H_{\mathscr{D}\breve{\mathscr{H}}} + iH_{\breve{Q}})^2 xyz\dot{z} = 0. \tag{6.60}$$

The discriminant of this quadratic form in (xy) and $(z\dot{z})$ is

$$d = [H_{\mathscr{D}\mathscr{D}} H_{\breve{\mathscr{H}}\breve{\mathscr{H}}} - H_P{}^2 - ((H_{\mathscr{D}\breve{\mathscr{H}}} + iH_{\breve{Q}})^2]^2 + 4H_P{}^2 H_{\mathscr{D}\mathscr{D}} H_{\breve{\mathscr{H}}\breve{\mathscr{H}}} \geqslant 0. \tag{6.61}$$

Defining

$$\begin{matrix}\tau \\ \mu\end{matrix}\Big] := \frac{1}{2H_P}\{\sqrt{d} \pm [H_P{}^2 + (H_{\mathscr{D}\breve{\mathscr{H}}} + iH_{\breve{Q}})^2 - H_{\mathscr{D}\mathscr{D}} H_{\breve{\mathscr{H}}\breve{\mathscr{H}}}]\} \tag{6.62}$$

and supposing $H_{\breve{\mathscr{H}}\breve{\mathscr{H}}} \neq 0$, the determinant becomes

$$\Delta = \frac{H_P}{H_{\breve{\mathscr{H}}\breve{\mathscr{H}}}}(H_{\breve{\mathscr{H}}\breve{\mathscr{H}}} xy - \tau z\dot{z})(H_{\breve{\mathscr{H}}\breve{\mathscr{H}}} xy + \mu z\dot{z}). \tag{6.63}$$

We claim that τ is strictly positive when $H_P > 0$, independent of the values of the other derivatives of H. To prove the assertion assume $\tau \leqslant 0$; then $\sqrt{d} \geqslant 0$ implies

$$\lambda := H_P{}^2 + (H_{\mathscr{D}\breve{\mathscr{H}}} + iH_{\breve{Q}})^2 - H_{\mathscr{D}\mathscr{D}} H_{\breve{\mathscr{H}}\breve{\mathscr{H}}} \leqslant 0. \tag{6.64}$$

The definition of d and $\tau \leqslant 0$ necessitates $\sqrt{d} \leqslant -\lambda \to d = \lambda^2$. Since $H_P \neq 0$ this requires

$$H_P{}^2 + (H_{\mathscr{D}\breve{\mathscr{H}}} + iH_{\breve{Q}})^2 \leqslant \lambda \leqslant 0 \to H_P = 0, \tag{6.65}$$

which is a contradiction of the assumption $H_P > 0$. Therefore $\tau > 0$ and the determinant can be factored such that

$$\Delta = (H_P/\tau)(H_{\mathscr{P}\mathscr{P}}xy - \tau z\dot{z})(\tau xy + H_{\mathscr{D}\mathscr{D}}z\dot{z}). \tag{6.66}$$

Although it was originally assumed that $H_{\mathscr{P}\mathscr{P}} \neq 0$, the result remains valid when $H_{\mathscr{P}\mathscr{P}} \to 0$ because, in the final result, this derivative has disappeared from the denominators. When the background field is algebraically general, the two equations for the characteristic surfaces, obtained from $\Delta = 0$, are

$$\text{I: } \tau xy + H_{\mathscr{D}\mathscr{D}}z\dot{z} = 0 \quad \text{and} \quad \text{II: } H_{\mathscr{P}\mathscr{P}}xy - \tau z\dot{z} = 0. \tag{6.67}$$

These equations are linearly dependent if and only if $d = 0$. Using (6.58), these may be rewritten into the two alternative characteristic types,

$$\begin{aligned} &\text{I: } (\tau - H_{\mathscr{D}\mathscr{D}})\Sigma + (1/|Z|)(H_{\mathscr{D}\mathscr{D}} + \tau)\tau^{\mu\nu}S_{;\mu}S_{;\nu} = 0, \\ &\text{II: } (H_{\mathscr{P}\mathscr{P}} + \tau)\Sigma + (1/|Z|)(H_{\mathscr{P}\mathscr{P}} - \tau)\tau^{\mu\nu}S_{;\mu}S_{;\nu} = 0. \end{aligned} \tag{6.68}$$

As a consistency criteria, (6.68) for null background fields must reduce to (6.45) by the limiting transition $Z = P + \breve{Q} \to 0$ (i.e., $\mathscr{D} + i\breve{\mathscr{H}} \to 0$). Applying the correspondence condition in the limit, τ becomes unity and the coefficients of the characteristic equations conform to the conclusion

$$\begin{aligned} &\text{if } H_{PP} + H_{\breve{Q}\breve{Q}} \geqslant 0,\ I \to P \text{ and } II \to \breve{Q}, \\ &\text{if } H_{PP} + H_{\breve{Q}\breve{Q}} \leqslant 0,\ I \to \breve{Q} \text{ and } II \to P. \end{aligned} \tag{6.69}$$

The linearly dependent case, $d = 0$, occurs if and only if

$$H_{\mathscr{D}\mathscr{P}} + iH_{\breve{Q}} = 0 = H_{\mathscr{D}\mathscr{D}}H_{\mathscr{P}\mathscr{P}} + H_P^2. \tag{6.70}$$

Under these conditions $\tau = H_P$, reducing both characteristic equations for the single surface to

$$H_{\mathscr{P}\mathscr{P}}xy - H_P z\dot{z} = 0 \leftrightarrow H_P xy + H_{\mathscr{D}\mathscr{D}}z\dot{z} = 0 \tag{6.71}$$

or

$$(H_{\mathscr{P}\mathscr{P}} + H_P)\Sigma + (1/|Z|)(H_{\mathscr{P}\mathscr{P}} - H_P)\tau^{\mu\nu}S_{;\mu}S_{;\nu} = 0. \tag{6.72}$$

From some straight forward algebraic manipulation of (6.70), (6.71), (6.59), and (6.61), one deduces

$$d = 0 \leftrightarrow \rho = 0 = \sigma. \tag{6.73}$$

Therefore, with $d = 0$, (6.36) holds indentically for any $\Delta w \neq 0$, and ΔP_{AB} from (6.34) contains two arbitrary constants (the real and imaginary parts of Δw). If we assume $H_{\mathscr{P}\mathscr{P}} > 0$ and calculate $4\Delta P_{AB}\Delta P^{AB}$, we again determine that this invariant cannot vanish and remain consistent with the characteristic equation (6.71). Consequently, $\Delta P_{\mu\nu}$ is an algebraically general (but simple) bivector. Notice that a positive sign for $H_{\mathscr{P}\mathscr{P}}$ is not unexpected for a reasonable structure function since correspondence requires it for sufficiently small invariants.

Assume now $d \neq 0$; then Δ factors into two linear forms which are not proportional, giving two distinct characteristic equations of the form (6.67) where the coefficients are all real. Suppose that the integral of at least one equation, say the second, is GCS (i.e., $\tau \neq H_{\mathscr{P}\mathscr{P}}$ or $xy - z\dot{z} \neq 0$). Because of (6.73) and (6.38), $d \neq 0 \to |\rho| = |\sigma| \neq 0$, and Δw has the form

$$\Delta w = \Delta\lambda e^{(i/2)\arg(-\sigma/\rho)}, \tag{6.74}$$

with $\Delta\lambda$ real, arbitrary, and nonzero. From (6.34), ΔP_{AB} contains only one arbitrary parameter $\Delta\lambda$ fixing the phase. Analogously to the previous cases, for GCS with $d \neq 0$ the expression $4\Delta P_{AB}\Delta P^{AB}$ is nonvanishing, so that $\Delta P_{\mu\nu}$ is an algebraically general (but simple) bivector.

When the background field is algebraically general ($P_{AB} = -\frac{1}{2}(\mathscr{D} + i\breve{\mathscr{H}})k_{(A}l_{B)}$), (6.42) can be rewritten in the form

$$\begin{aligned} \Delta C_{ABCD} = {} & 4H_P\Sigma^{-1}\dot{Z}\Delta\dot{w}[x^2z^2k_Ak_Bk_Ck_D + y^2\dot{z}^2l_Al_Bl_Cl_D \\ & + 2(xy + z\dot{z})(xzk_{(A}k_Bk_Cl_{D)} + y\dot{z}l_{(A}l_Bl_Ck_{D)}) \\ & + (x^2y^2 + 4xyz\dot{z} + z^2\dot{z}^2)k_{(A}k_Bl_Cl_{D)})] \\ & + 4H_P\Sigma Z\Delta w k_{(A}k_Bl_Cl_{D)}. \end{aligned} \tag{6.75}$$

If the characteristics satisfy the second of (6.67) or are of type II, the invariants are

$$z = ((H_{\mathscr{P}\mathscr{P}}/\tau)xy)^{1/2}e^{i\phi}, \quad \Sigma = (H_{\mathscr{P}\mathscr{P}}/\tau - 1)xy. \tag{6.76}$$

Defining $H_{\mathscr{P}\mathscr{P}}/\tau := \xi$, the conformal curvature jump is

$$\begin{aligned} \Delta C_{ABCD} = {} & 4H_P(\xi - 1)^{-1}\dot{Z}\Delta\dot{w}[\xi(x^2e^{2i\phi}k_Ak_Bk_Ck_D + y^2e^{-2i\phi}l_Al_Bl_Cl_D) \\ & + 2(1 + \xi)\xi^{1/2}(x^{3/2}y^{1/2}e^{i\phi}k_{(A}k_Bk_Cl_{D)} + x^{1/2}y^{3/2}e^{-i\phi}l_{(A}l_Bl_Ck_{D)}) \\ & + (1 + 4\xi + \xi^2)xyk_{(A}k_Bl_Cl_{D)}] + 4H_P(\xi - 1)Z\Delta w xyk_{(A}k_Bl_Cl_{D)}. \end{aligned} \tag{6.77}$$

Defining $\tilde{k}_A := e^{i\phi/2}x^{1/2}k_A, \tilde{l}_A = e^{-i\phi/2}y^{1/2}l_A \to \tilde{k}^A\tilde{l}_A = (xy)^{1/2}$, and $\eta_A := (xy)^{-1/2}(\tilde{k}_A + \eta\tilde{l}_A) \to \tilde{k}^A\eta_A = \eta$, $\tilde{l}^A\eta_A = -1$, (6.77) can be transformed into an expression which has a characteristic polynomial of the form

$$\Delta C_{ABCD}\eta^A\eta^B\eta^C\eta^D = 4H_P(\xi - 1)^{-1}\dot{Z}\Delta\dot{w}[\xi(\eta^4 + 1) - 2(1 + \xi)\xi^{1/2}(\eta^3 + \eta) + (1 + 4\xi + \xi^2)\eta^2] + 4H_P(\xi - 1)Z\Delta w\eta^2 = 0, \tag{6.78}$$

which has the distinct roots

$$\begin{aligned} \eta_{\pm\pm} = {} & \tfrac{1}{2}\xi^{-1/2}\{(1 + \xi) \pm i(\xi - 1)[Z\Delta w/\dot{Z}\Delta\dot{w} + 2\xi(\xi - 1)^{-2}]^{1/2}\} \\ & \pm [\tfrac{1}{4}\xi^{-1}\{(1 + \xi) \pm i(\xi - 1)[Z\Delta w/\dot{Z}\Delta\dot{w} + 2\xi(\xi - 1)^{-2}]^{1/2}\}^2 - 1]^{1/2}. \end{aligned} \tag{6.79}$$

Therefore, ΔC_{ABCD} is of type I:[1 - 1 - 1 - 1].

Similarly, if the characteristics are of type I,

$$x=(-(H_{\mathscr{O}\mathscr{O}}/\tau)z\dot{z})^{1/2}e^{\omega},\quad y=(-(H_{\mathscr{O}\mathscr{O}}/\tau)z\dot{z})^{1/2}e^{-\omega},$$
$$\Sigma=(1+H_{\mathscr{O}\mathscr{O}}/\tau)z\dot{z}, \tag{6.80}$$

where ω is real. Defining $\tilde{k}_A=e^{\omega/2}z^{1/2}k_A$, $\tilde{l}_A=e^{-\omega/2}\dot{z}^{1/2}l_A\to\tilde{k}^A\tilde{l}_A=(z\dot{z})^{1/2}$, one obtains the same result for the jump except for an overall change of sign and an interchange of $H_{\mathscr{X}\mathscr{X}}$ with $-H_{\mathscr{O}\mathscr{O}}$; and ΔC_{ABCD} is also of type I:[1-1-1-1].

For GCS, each jump expression for the conformal curvature [specifically (6.42) and its consequences (6.54) and (6.75)] becomes to conformally flat when the perturbation in the electrodynamic field vanishes. When this circumstance occurs or, that is, when $\Delta w=0$, (6.42) requires

$$\Sigma\Delta C_{ABCD}=0\to\begin{cases}\Delta C_{ABCD}=0 \text{ if } \Sigma\neq 0\\ \Delta C_{ABCD} \text{ is of type } N\text{:}[4] \text{ if } \Sigma=0\end{cases} \tag{6.81}$$

Therefore, whenever there exists a nonvanishing discontinuous jump in the perturbation of the conformal curvature with $\Delta w=0$, the jump is of type N:[4] and the characteristic surfaces have degenerated to NCS. Certainly, for this subcase the number of free parameters in the jump also returns to the values appropriate for the corresponding NCS.

7. METRIC PROPERTIES OF GENERAL CHARACTERISTIC SURFACES

For general characteristic surfaces ($\Sigma\neq 0$), the conditions distinguishing the surfaces $S(x)=0$ as timelike with spacelike gradient ($\Sigma>0$) or spacelike with timelike gradient ($\Sigma<0$) are now investigated. Under the first circumstance the characteristic cones are interpreted as being inside of the standard cone, and in the second as outside. Certain structure function properties can permit the propagation of discontinuities of the derivatives in excess of the "speed of light". For convenience, we introduce the following notation: $CS\equiv$ characteristic surface, $T\equiv$ timelike, $S\equiv$ spacelike, and $N\equiv$ lightlike or null.

A. Analyzing GCS with null background electrodynamic field

$P_{AB}=\frac{1}{4}Pk_Ak_B\to\tau_{\mu\nu}=|P|^2k_\mu k_\nu$. $k^\mu k_\mu=0$, we infer from (6.45) that

$$P\text{: } \Sigma=-H_{PP}|P|^2(k_\mu S^{,\mu})^2,$$
$$\breve{Q}\text{: } \Sigma=H_{\breve{Q}\breve{Q}}|P|^2(k_\mu S^{,\mu})^2. \tag{7.1}$$

Consequently,

$$\text{CS of type } P \text{ is } \begin{cases}T & \text{if} \quad H_{PP}<0\\ N & \quad H_{PP}=0\\ S & \quad H_{PP}>0\end{cases} \tag{7.2a}$$

$$\text{CS of type } \breve{Q} \text{ is } \begin{cases}T & \text{if} \quad H_{\breve{Q}\breve{Q}}>0\\ N & \quad H_{\breve{Q}\breve{Q}}=0\\ S & \quad H_{\breve{Q}\breve{Q}}<0.\end{cases} \tag{7.2b}$$

B. For GCS with an algebraically general background field where $-\Sigma=xy-z\dot{z}$, types I and II of (6.67) are decomposed separately

Introducing the definitions

$$X:=H_{P\breve{Q}}{}^2-H_{PP}H_{\breve{Q}\breve{Q}},$$
$$Y:=(H_{\mathscr{X}\mathscr{X}}-H_P)(H_{\mathscr{O}\mathscr{O}}+H_P)-(H_{\mathscr{O}\mathscr{X}}+iH_{\breve{Q}})^2$$
$$=4|Z|^2X, \tag{7.3}$$

$X\neq 0$ assures that neither of (6.67) can reduce to $xy-z\dot{z}=0$, or null surfaces can occur only in the exceptional situation where simultaneously $xy=0=z\dot{z}$.

For characteristics of type I from (6.67),

$$\tau xy+H_{\mathscr{O}\mathscr{O}}z\dot{z}=0\Leftrightarrow\Sigma=(H_{\mathscr{O}\mathscr{O}}/\tau+1)z\dot{z}, \tag{7.4}$$

where

$$\text{CS is } T\Leftrightarrow -H_{\mathscr{O}\mathscr{O}}/\tau-1<0. \tag{7.5a}$$

CS with (I) $-H_{\mathscr{O}\mathscr{O}}>0$ is

(a) T if $\tau>-H_{\mathscr{O}\mathscr{O}}$

and $\begin{cases}Y-H_p(H_{\mathscr{X}\mathscr{X}}+H_{\mathscr{O}\mathscr{O}})<0 \text{ or}\\ [Y-H_p(H_{\mathscr{X}\mathscr{X}}+H_{\mathscr{O}\mathscr{O}})\geqslant 0 \text{ and } Y<0].\end{cases}$

(b) S if $Y>0$.

(II) $-H_{\mathscr{O}\mathscr{O}}<0$ is T. (7.5b)

$$\text{CS is } S\Leftrightarrow -H_{\mathscr{O}\mathscr{O}}/\tau-1>0\Leftrightarrow -H_{\mathscr{O}\mathscr{O}}>0 \text{ and}$$
$$\tau<-H_{\mathscr{O}\mathscr{O}} \text{ with}$$

(I) $Y>0\Leftrightarrow X>0$ for $Z\neq 0$ and/or

(II) $Y-H_P(H_{\mathscr{X}\mathscr{X}}+H_{\mathscr{O}\mathscr{O}})>0$. (7.5c)

$$\text{CS is } N\Leftrightarrow -H_{\mathscr{O}\mathscr{O}}=\tau. \tag{7.5d}$$

For characteristics of type II from (6.67),

$$H_{\mathscr{X}\mathscr{X}}xy-\tau z\dot{z}\Leftrightarrow\Sigma=-(\tau/H_{\mathscr{X}\mathscr{X}}-1)z\dot{z}, \tag{7.6}$$

where

$$\text{CS is } T\Leftrightarrow\tau/H_{\mathscr{X}\mathscr{X}}-1<0. \tag{7.7a}$$

CS with (I) $H_{\mathscr{X}\mathscr{X}}<0$ is T.

(II) $H_{\mathscr{X}\mathscr{X}}>0$ is (a) $T\Leftrightarrow\tau<H_{\mathscr{X}\mathscr{X}}\Leftrightarrow Y+H_p(H_{\mathscr{X}\mathscr{X}}+H_{\mathscr{O}\mathscr{O}})>0\Rightarrow Y>0\Leftrightarrow X>0$ for $Z\neq 0$.

(b) S if $Y<0$. (7.7b)

$$\text{CS is } S\Leftrightarrow\tau/H_{\mathscr{X}\mathscr{X}}-1>0\Leftrightarrow\tau>H_{\mathscr{X}\mathscr{X}}, \text{ which follows if} \tag{7.7c}$$

(I) $Y+H_P(H_{\mathscr{X}\mathscr{X}}+H_{\mathscr{O}\mathscr{O}})<0$ or

(II) $Y+H_P(H_{\mathscr{X}\mathscr{X}}+H_{\mathscr{O}\mathscr{O}})\geqslant 0$ and $Y<0$.

$$\text{CS is } N\Leftrightarrow\tau=H_{\mathscr{X}\mathscr{X}}. \tag{7.7d}$$

In synthesis we deduce

$$\{\text{I and II are } T \text{ and } H_{\mathscr{X}\mathscr{X}}>0,\ -H_{\mathscr{O}\mathscr{O}}>0\}$$
$$\Rightarrow\{H_P(H_{\mathscr{O}\mathscr{O}}+H_{\mathscr{X}\mathscr{X}})>Y>0\}, \tag{7.8a}$$

$$\{\text{I is } S \text{ and II is } T,$$
$$H_{\mathscr{X}\mathscr{X}}>0\}\Rightarrow\{-H_{\mathscr{O}\mathscr{O}}>0$$
and
$$Y>H_P|H_{\mathscr{O}\mathscr{O}}+H_{\mathscr{X}\mathscr{X}}|>0\}, \tag{7.8b}$$

$$\{\text{I is } T \text{ and II is } S,$$
$$-H_{\mathscr{O}\mathscr{O}}>0\}\Rightarrow\{H_{\mathscr{X}\mathscr{X}}>0 \text{ and } -Y>0\}, \tag{7.8c}$$

$$\{\text{I and II are } S\} \Rightarrow \{H_{\mathscr{K}\mathscr{K}} > 0,\ -H_{\mathscr{D}\mathscr{D}} > 0 \text{ and } -H_P(H_{\mathscr{D}\mathscr{D}} + H_{\mathscr{K}\mathscr{K}}) > Y > 0\}. \tag{7.8d}$$

The conditions for the four alternatives (7.8) are mutually exclusive; therefore, they are not only necessary but also sufficient and the implication $\Rightarrow$ may be replaced by $\Leftrightarrow$ in each. Notice, finally, that discontinuities of the derivatives of small perturbations of the nonlinear electrodynamic field are propagated within the light cone if and only if (7.8) is satisfied, which is equivalent to

$$(H_P/2|Z|)(H_{PP} - H_{\breve{Q}\breve{Q}}) > H_{P\breve{Q}}{}^2 - H_{PP}H_{\breve{Q}\breve{Q}} > 0. \tag{7.9}$$

In the case where $d = 0$ the surfaces coincide, and the resultant conditions may be read from (7.5) and (7.7) by recalling that $\tau = H_P$ for this situation. There are of course other special cases, for example, a complete set where one characteristic surface is null and (6.15) necessitates that $X = 0$. But a detailed investigation of these generally pathologic cases would be excessive pedantry, since a sufficient number of relevant cases has already been displayed.

Next we reconsider the eiconal equation $\gamma^{\mu\nu}S_{,\mu}S_{,\nu} = 0$ for GCS, where nonlinear electrodyamic waves are transported along bicharacteristic rays which are null with respect to the metric $\gamma^{\mu\nu}$ as opposed to $g^{\mu\nu}$. Directly from the characteristic surface equations (6.45), for the case of a null electromagnetic field, the eiconal equation implies

$$\begin{aligned} P\text{:}\ & \gamma^{(P)\mu\nu} = \phi^{-2}(g^{\mu\nu} + H_{PP}\tau^{\mu\nu}) \\ \breve{Q}\text{:}\ & \gamma^{(\breve{Q})\mu\nu} = \phi^{-2}(g^{\mu\nu} - H_{\breve{Q}\breve{Q}}\tau^{\mu\nu}), \end{aligned} \tag{7.10}$$

where ϕ is an arbitrary conformal factor. As a note, these metrics coincide if and only if the structure function is the Hamiltonian of Born–Infeld NLE.[2] Also from (6.68), for the case of an algebraically general electromagnetic field, the eiconal equation implies

$$\text{I: } \gamma^{(I)\mu\nu} = \phi^{-2}\left[g^{\mu\nu} + \frac{1}{|Z|}(H_{\mathscr{D}\mathscr{D}} + \tau)/(\tau - H_{\mathscr{D}\mathscr{D}})\,\tau^{\mu\nu}\right], \tag{7.11}$$

$$\text{II: } \gamma^{(II)\mu\nu} = \phi^{-2}\left[g^{\mu\nu} + \frac{1}{|Z|}(H_{\mathscr{K}\mathscr{K}} - \tau)/(H_{\mathscr{K}\mathscr{K}} + \tau)\tau^{\mu\nu}\right].$$

The sum of the coefficients in (7.11) contains the multiplicative factor $H_{PP} - H_{\breve{Q}\breve{Q}}$, which vanishes in the case of analytic NLE; therefore, for this subcase

$$\text{I, II:} \gamma^{(A)\mu\nu} = \phi^{-2}[g^{\mu\nu} \mp (H_{\mathscr{K}\mathscr{K}} - \tau)/(H_{\mathscr{K}\mathscr{K}} + \tau)\tau^{\mu\nu}]. \tag{7.12}$$

These metrics coincide when the discriminant d vanishes and the metric is (7.12) with $\tau = H_P$.

The intent of writing the metrics in these explicit forms is to make apparent their common structure. Each appears as

$$\gamma^{\mu\nu} = \phi^{-2}(g^{\mu\nu} + F(P,\breve{Q})\tau^{\mu\nu}), \tag{7.13}$$

where $g^{\mu\nu}$ is the Einsteinian metric whose geodesics are the trajectories of gravitons, $F(P,\breve{Q})$ is a function of the invariants of the electrodynamic field $P^{\mu\nu}$ and $\tau^{\mu\nu}$ is the traceless energy–momentum tensor constructed from $P^{\mu\nu}$. Due to the presence of the conformal factor ϕ, a gauge can always be chosen such that only the conformally invariant part is relevant to the geodesics of $\gamma^{\mu\nu}$ or, specifically, to the trajectories of the nonlinear photons. Perhaps the more curious physical situations occur when the metric $\gamma^{\mu\nu}$ is such that its corresponding null cone is exterior to that of $g^{\mu\nu}$ as specified in the constraints (7.2), (7.5), and (7.7), because these cases permit for the extraordinary speeds of interaction.

8. CONCLUSION

The dynamic equations for a charged perfect fluid with nonlinear electrodynamic interaction in a gravitational space–time are deduced from the fundamental action. The characteristic surfaces for this physical system are found to have discontinuous first derivatives of small perturbations in the fields (1) which may be of general types and (2) which

TABLE I. Types of discontinuous jumps.

Characteristic equations	Restrictions on H	$\Delta P_{\mu\nu}$	Limit	No. of parameters in $\Delta P_{\mu\nu}$	$\Delta C_{\mu\nu\lambda\kappa}$	No. of parameters in $\Delta C_{\mu\nu\lambda\kappa}$
$\Sigma = 0$	$H = P$	[2]	$\Delta f \to 0$	$2 \to 0$	[3-1]$\to$[4]	$4 \to 2$
$\Sigma = 0$ $P^{\beta}_{\alpha}S_{,\beta} \neq \lambda S_{,\alpha}$	$\Delta H_z = 0$					
	(a)$H_{ZZ} = H_{Z\dot{Z}} = 0$	[2]	$\Delta P' \to 0$	$2 \to 0$	[3-1]$\to$[4]	$4 \to 2$
	(b)$\lvert H_{ZZ}\rvert = \lvert H_{Z\dot{Z}}\rvert \neq 0$	[2]	$\Delta P' \to 0$	$1 \to 0$	[3-1]$\to$[4]	$3 \to 2$
$P^{\beta}_{\alpha}S_{,\beta} = \lambda S_{\alpha}, H_{\mathscr{K}\mathscr{K}} = 0$	$\Delta H_z \neq 0$	[1-1]	$\Delta P' \to 0$	$3 \to 1$	[2-1-1]$\to$[2,2]	$5 \to 3$
					$D = 0$ [3-1]$\to$[4]	$4 \to 2$
			$\Delta P \to 0$	$3 \to 2$	[2-1-1]$\to$[3,1]	$5 \to 4$
					$D - i\mathscr{K} = 0$ [2,2]$\to$[4]	$3 \to 2$
			$\begin{Bmatrix}\Delta P'\\ \Delta P\end{Bmatrix} \to 0$	$3 \to 0$	[2-1-1]$\to$[4]	$5 \to 2$
$P\text{:}\Sigma + H_{PP}\tau^{\mu\nu}S_{,\mu}S_{,\nu} = 0$	$H_{PP} + H_{\breve{Q}\breve{Q}} \neq 0$	[1-1]	$\Delta w \to 0$	$1 \to 0$	[1-1-1-1]$\to$[-]	$1 \to 0$
$\breve{Q}\text{:}\Sigma - H_{\breve{Q}\breve{Q}}\tau^{\mu\nu}S_{,\mu}S_{,\nu} = 0$	$H_{PP} + H_{\breve{Q}\breve{Q}} = 0$					
	P coincides with $\breve{Q}$	(1-1]	$\Delta w \to 0$	$2 \to 0$	[1-1-1-1]$\to$[-]	$2 \to 0$
I: $\tau xy + H_{\mathscr{D}\mathscr{D}}z\dot{z} = 0$	$d \neq 0$	[1-1]	$\Delta w \to 0$	$1 \to 0$	[1-1-1-1]$\to$[-]	$1 \to 0$
II: $H_{\mathscr{K}\mathscr{K}}xy - \tau z\dot{z} = 0$	$d = 0$					
	I coincides with II	[1-1]	$\Delta w \to 0$	$2 \to 0$	[1-1-1-1]$\to$[-]	$2 \to 0$

could have spacelike propagation. These perhaps unexpected properties are entirely dependent upon the specific nature of the structure function of the nonlinearity. Presumably, the introduction of other nonlinear interactions (e.g., fluid dynamic) could be anticipated to provide similar consequences. The demonstration of a physically relevant source for a nonlinear electrodynamic interaction providing causal spacelike signal propagation remains open. However, spacelike quantum processes present possible candidates. Permitting for curved gravitational space–times and for characteristic surfaces under various restrictions, the discontinuous jumps generated are cataloged in Table I. In each case, the procedure for limiting to a vanishing electrodynamic jump is also presented.[22] A speculative comment on the emergence of conformal curvature jumps of type I: [1-1-1-1] is perhaps appropriate. The nonvanishing trace of the energy–momentum tensor [since $-\frac{1}{4}R = \lambda + 2(ZH_Z + \dot{Z}H_{\dot{Z}} - H)$] implies the existence of some finite fundamental mass and, consequently, length which ought to force the breaking of the conformal group previously enjoyed by the electrodynamic equations in the linear case. Under these circumstances, jumps of general types are not implausible.

Whenever the characteristic surfaces are of types P and $\check{Q}$, the discontinuities in the derivatives of small perturbations of the nonlinear electrodynamic field are propagated interior to the light cone if and only if $H_{PP} < 0 < H_{\check{Q}\check{Q}}$.

For characteristic surfaces of types I and II, the discontinuities are propagated within the light cone if and only if

$$(H_P/2|Z|)(H_{PP} - H_{\check{Q}\check{Q}}) > H_{P\check{Q}}{}^2 - H_{PP}H_{\check{Q}\check{Q}} > 0.$$

Consequently, if the physical environment is sufficiently nonlinear, there exists a distinct chance that there are relevant structure functions permitting spacelike propagation of jumps of general types.

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[16]The dual is defined for a tensor of rank n by

$$\check{T}^{\mu_1\cdots\mu_4}{}_{\nu_1\cdots\nu_n} := \frac{1}{2(-g)^{1/2}}\, e^{i(\pi/2)[n(4-n)]}\, \frac{1}{4!}\epsilon^{\mu_1\cdots\mu_4}{}_{\nu_1\cdots\nu_n}\epsilon^{\nu_1\cdots\nu_n}{}_{\lambda_1\cdots\lambda_n} T_{\lambda_1\cdots\lambda_n}$$

such that $\check{\check{T}}\cdots = T\cdots$.

[17]A pseudoinvariant, under C_∞ transformations, transforms like a scalar times the sign $[\partial(x)/\partial(x')]$.

[18]The conventions of J. F. Plebañski, "Spinors, Tetrads, and Forms," a monograph in two volumes of the Centro de Investigación y de Estudios Avanzados del IPN, México (1975) are generally observed. Index, differentiation, and symmetrization symbols are conventional. The sign: = (equal from definition) is distinguished from = (equal due to logic).

The curvature tensor

$$R^{\alpha}{}_{\beta\gamma\delta} := -\left\{{}^{\alpha}_{\beta\gamma}\right\}_{,\delta} + \left\{{}^{\alpha}_{\beta\delta}\right\}_{,\gamma} + \left\{{}^{\alpha}_{\sigma\gamma}\right\}\left\{{}^{\sigma}_{\beta\delta}\right\} - \left\{{}^{\alpha}_{\sigma\delta}\right\}\left\{{}^{\sigma}_{\beta\gamma}\right\}$$

induces the Ricci tensor and scalar curvature

$$R_{\alpha\beta} = R^{\rho}{}_{\alpha\rho\beta} \text{ and } R = g^{\alpha\beta}R_{\alpha\beta}.$$

The Einstein and conformal curvature tensors are defined, respectively, by

$$G_{\alpha\beta} := R_{\alpha\beta} - \tfrac{1}{2}g_{\alpha\beta}R$$

and

$$R^{\alpha\beta}{}_{\gamma\delta} = :C^{\alpha\beta}{}_{\gamma\delta} + \tfrac{1}{2}\delta^{\alpha\beta\rho}_{\gamma\delta\sigma}\left(R^{\sigma}_{\rho} - \tfrac{1}{4}\delta^{\sigma}_{\rho}R\right) + \tfrac{1}{12}\delta^{\alpha\beta}_{\gamma\delta}R.$$

[19]The relation between the metric and the matrices is

$$g_{\mu\nu} = -\tfrac{1}{2}\epsilon^{AC}\epsilon^{\dot{B}\dot{D}}g_{\mu A\dot{B}}g_{\nu C\dot{D}},$$

and the spin tensor is defined by

$$S^{\mu\nu AB} := \tfrac{1}{2}\epsilon_{\dot{R}\dot{S}}(g^{\mu A\dot{R}}g^{\nu B\dot{S}} - g^{\nu A\dot{R}}g^{\mu B\dot{S}}).$$

[20]J. F. Plebañski, "Non-linear Electrodynamics, a Study", monograph of the Centro de Investigación y de Estudios Avanzados del IPN, México (1966).

[21]These vectors can be defined and oriented such that

$$E^{\alpha} = f^{\alpha}{}_{\beta}n^{\beta}, \check{B}^{\alpha} = -i\check{f}^{\alpha}_{\beta}n^{\beta},$$

$$D^{\alpha} = P^{\alpha}{}_{\beta}n^{\beta}, \check{H}^{\alpha} = -i\check{P}^{\alpha}{}_{\beta}n^{\beta},$$

for any n^{β} with $n^{\beta}n_{\beta} = -1$ and $n_4 > 0$.

[22]The appearance of [-] rather than [4] and the seemingly unusual number of parameters in $\Delta C_{\mu\nu\lambda\kappa}$ for the GCS results from (6.81).

Partitioning lower bounds for Bubnov–Galerkin's eigenvalues [a)]

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(Received 4 November 1980; accepted for publication 19 June 1981)

Löwdin's partitioning technique is extended for calculating energy lower bounds in Bubnov–Galerkin's eigenvalue problems.

PACS numbers: 03.65.Ca

1. INTRODUCTION

The Alexander Weinstein treatment [or the method of intermediate operators (MIO)[1–3]] of Rayleigh–Ritz eigenvalue problems (RREP[4–7]), i.e.,

$$H|\psi\rangle = E|\psi\rangle, \tag{1}$$

provided us with an approach for determining lower bounds on the eigenvalues E of such problems. The method was successfully tested, on the one hand, by many authors (see, e.g., Aronszajn,[8–10] Gould,[11] Weinstein and Stenger,[12] Weinberger,[13,14] and the references therein) in various fields of mathematical physics. It has been extended, on the other hand, to quantum mechanical problems through the original works of Bazley[15,16] and Bazley and Fox[17,18] using an adequate choice of the so-called reference-space (see also Ref. 12, Sec. 4). (Other choices of this space were suggested, later on, by Gay[19] and Miller[20]). However, several authors[21–25] have introduced a fundamentally different procedure for obtaining energy-lower bounds in the above mentioned problems. Their principal idea arose from a well known approach in the theory of determinants and matrices[26] called the partioning technique (PT). Both the MIO and the PT have been further simplified by Löwdin,[27–32] in his extensive works on perturbation theory, using different characteristics of operators in Hilbert space. Nevertheless, deep analysis of the two procedures has clarified some relations between their energies (see, e.g., Wilson[33]). Moreover, Löwdin and others[31–38] pointed out that these procedures can be employed, in addition to the Rayleigh–Ritz variational method, for calculating energies of arbitrary small errors. Contrary to RREP, the Bubnov–Galerkin's eigenvalue problems (BGEP), i.e.,

$$H_1|\psi\rangle = EH_2|\psi\rangle, \tag{2}$$

has awarded less interest in the literature of mathematical and theoretical physics. In fact, the importance of BGEP in the quantum theory has been stressed (especially in quantum chemistry) by many authors (see, e.g., Hall,[39] Hall *et al*,[40,41] Robinson and Epstein,[42] and Thulstrup *et al.*[43]). A variational treatment of Eq. (2), however, was discussed explicitly, many years ago, by Bubnov and Galerkin (see Michlin[44]). Their approach leads to energies of similar qualities as those obtained by the Rayleigh–Ritz method, i.e., to upper bounds on the exact eigenvalues E. Moreover, quadratic variational methods, analogous to those of James and Coolidge[45] and Preuss[46] as well as Frost's method,[47] were demonstrated very recently by Abdel-Raouf[48] for dealing with the same problems.

On the other hand, energy-lower bounds for BGEP have been represented by Aronszajn[49] and Bazely[15] (see also Weinberger,[14] Chap. 4) within the framework of the method of intermediate operators. These bounds, however, are associated with difficulties in constructing and treating the "base problem," the intermediate problems, as well as the reference-space. The present work is devoted to the formulation of energy-lower bounds for BGEP using Löwdin's partioning technique. We start by employing matrix representation and proceed steadily towards an abstract formalism for the lower bounds.

2. PARTITIONING OF MATRICES

In the variational treatment of BGEP [Eq. (2)], one considers that the vector $|\psi\rangle$ is the superposition of a complete set of Hilbert-space vectors $\{|\chi_i\rangle\}$, i.e.,

$$|\psi\rangle = \sum_i c_i|\chi_i\rangle. \tag{3}$$

Substitution from Eq. (3) into Eq. (2) leads, after varying the parameters, to the conventional secular equations

$$\sum_j \{\langle\chi_i|H_1|\chi_j\rangle - E\langle\chi_i|H_2|\chi_j\rangle\}c_j = 0, \quad i = 1,2,\ldots \tag{4}$$

characteristic of the variational theory. In Eqs. (4), it is assumed that H_1 and H_2 are Hermitian operators. This system of equations can be abbreviated into the form

$$Ac = EBc, \tag{5}$$

where the matrices A and B possess the following elements, respectively:

$$A_{ij} = \langle\chi_i|H_1|\chi_j\rangle, \tag{6a}$$

$$B_{ij} = \langle\chi_i|H_2|\chi_j\rangle, \tag{6b}$$

and the column vector c is defined by

$$c = \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix}. \tag{6c}$$

We now assume that the set $\{|\chi_i\rangle\}$ is partitioned into two parts $\{a\}$ and $\{b\}$ (where a and b represent also the number of elements in each part). Therefore Eq. (5) can be written in the form

$$\begin{pmatrix} A_{aa} & A_{ab} \\ A_{ba} & A_{bb} \end{pmatrix}\begin{pmatrix} c_a \\ c_b \end{pmatrix} = E\begin{pmatrix} B_{aa} & B_{ab} \\ B_{ba} & B_{bb} \end{pmatrix}\begin{pmatrix} c_a \\ c_b \end{pmatrix}. \tag{7}$$

[a)]Work supported by the Deutsche Forschungsgemeinschaft.

 0022-2488/81/122849-05$01.00

Thus we have the relations

$$A_{aa}c_a + A_{ab}c_b = E(B_{aa}c_a + B_{ab}c_b), \tag{8a}$$

$$A_{ba}c_a + A_{bb}c_b = E(B_{ba}c_a + B_{bb}c_b). \tag{8b}$$

The last equation gives the following value of c_b:

$$c_b = (EB_{bb} - A_{bb})^{-1}(A_{ba} - EB_{ba})c_a. \tag{9}$$

Substitution from Eq. (9) into Eq. (8a) leaves us with

$$\{EB_{aa} - A_{aa} - (A_{ab} - EB_{ab})(EB_{bb} - A_{bb})^{-1} \times (A_{ba} - EB_{ba})\}c_a = 0. \tag{10}$$

Consequently, we get, for all $c_a \neq 0$, the following implicit relation in E, namely:

$$E = B_{aa}^{-1}A_{aa} + B_{aa}^{-1}(A_{ab} - EB_{ab})(EB_{bb} - A_{bb})^{-1} \times (A_{ba} - EB_{ba}). \tag{11}$$

(Note that the square matrices A_{aa}, A_{bb}, B_{aa}, and B_{bb} are positive definite if and only if H_1 and H_2 are positive definite). Let us consider that the subset $\{a\}$ involves one vector $|\chi_1\rangle$ and that $c_1 \neq 0$. In this case Eq. (11) is reduced to the relation

$$E = f(E) = B_{11}^{-1}A_{11} + B_{11}^{-1}(A_{1b} - EB_{1b}) \times (EB_{bb} - A_{bb})^{-1}(A_{b1} - EB_{b1}), \tag{12}$$

which can be interpreted as E is equal to $B_{11}^{-1}A_{11}$ plus a perturbation term. [Notice the resemblance between Eqs. (12) and (15) in Ref. 24]. Choosing the vectors $|\chi_i\rangle$ to be H_2-orthonormal, i.e.,

$$\langle\chi_i|H_2|\chi_j\rangle = \delta_{ij} \quad \text{for all } i,j \tag{13}$$

we get

$$B_{1b} = B_{b1} = 0. \tag{14}$$

[Note that assumption (13) is always possible according to a corollary in Ref. 14, p. 40]. From Eqs. (12) and (14) we obtain the important relation

$$E = f(E) = B_{11}^{-1}\{A_{11} + A_{1b}(EB_{bb} - A_{bb})^{-1}A_{b1}\}, \tag{15}$$

which has the following derivative with respect to E:

$$\frac{\partial f(E)}{\partial E} = f'(E) = -B_{11}^{-1}A_{1b}(EB_{bb} - A_{bb})^{-1} \times B_{bb}(EB_{bb} - A_{bb})^{-1}A_{b1}. \tag{16}$$

However, from Eqs. (9) and (14), we get, at $a = 1$ and $c_1 \neq 0$, the values of c_b and c_b^+ by

$$c_b = (EB_{bb} - A_{bb})^{-1}A_{b1}c_1 \tag{17a}$$

and

$$c_b^+ = c_1^+A_{1b}(EB_{bb} - A_{bb})^{-1}. \tag{17b}$$

Therefore we have

$$c_b^+c_b/c_1^+c_1 = A_{1b}(EB_{bb} - A_{bb})^{-2}A_{b1}, \tag{18}$$

which is a positive quantity. Substitution from Eq. (18) into Eq. (16) leads to the valuable relation

$$f'(E) = -\frac{c_b^+B_{bb}c_b}{c_1^+B_{11}c_1} = -\frac{c_b^+c_b}{c_1^+c_1}, \tag{19}$$

which states that $f'(E)$ has a definite sign and the curve $f(E)$, E possesses, everywhere, negative inclination. From Eq. (15) we may define a function $F(E)$ such that

$$F(E) = E - f(E) = 0 \tag{20}$$

is valid. The derivative of this function satisfies the inequality

$$F'(E) = 1 - f'(E) > 0. \tag{21}$$

This emphasizes that Eqs. (2) and (20) have the same number of roots. The above characteristics of $f'(E)$, $F(E)$, and $F'(E)$ specify a rather favorable case for the calculus of iteration which may be treated using a method due to Newton and Raphson (see, e.g., Ref. 50, Secs. 71–80 and Ref. 51, Chap. 25). The iteration process converges if $|f'(E)| < 1$, i.e., if the inequality $c_b^+c_b < c_1^2$ is fulfilled. This happens if the vector $|\chi_1\rangle$ has a large contribution with $|\psi\rangle$ given by Eq. (3). Other properties of the energies obtained by Newton–Raphson's procedure are comprehensively discussed in the above mentioned works of Löwdin.

3. REFORMULATIONS USING PROJECTION MATRICES

Let us define two matrices Q and P by

$$Q = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad P = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \tag{22}$$

We note that Q and P are self-adjoint and satisfy the relations

$$Q + P = 1, \quad QP = PQ = 0. \tag{23}$$

Multiplication of Q and P with A (or B) and c of Eq. (7) provide us with the following matrices:

$$Qc = \begin{pmatrix} c_a \\ 0 \end{pmatrix}, \quad Pc = \begin{pmatrix} 0 \\ c_b \end{pmatrix}, \tag{24a}$$

$$QAQ = \begin{pmatrix} A_{aa} & 0 \\ 0 & 0 \end{pmatrix}, \tag{24b}$$

$$QAP = \begin{pmatrix} 0 & A_{ab} \\ 0 & 0 \end{pmatrix}, \tag{24c}$$

$$PAQ = \begin{pmatrix} 0 & 0 \\ A_{ba} & 0 \end{pmatrix}, \tag{24d}$$

and

$$PAP = \begin{pmatrix} 0 & 0 \\ 0 & A_{bb} \end{pmatrix}. \tag{24e}$$

Also we get from (24e) the matrix

$$P(EB - A)P = \begin{pmatrix} 0 & 0 \\ 0 & (EB_{bb} - A_{bb}) \end{pmatrix}. \tag{25}$$

However, from Eqs. (11) and (12) we notice that the matrix

$$T_{bb} = \begin{pmatrix} 0 & 0 \\ 0 & (EB_{bb} - A_{bb})^{-1} \end{pmatrix} \tag{26}$$

should appear in any generalized formulation of the technique presented in Sec. 2. For this reason we consider the equality

$$\begin{pmatrix} \alpha U_{aa} & 0 \\ 0 & (EB_{bb} - A_{bb}) \end{pmatrix}^{-1} = \begin{pmatrix} \alpha^{-1}U_{aa} & 0 \\ 0 & (EB_{bb} - A_{bb})^{-1} \end{pmatrix}, \tag{27}$$

which is true for all $\alpha \neq 0$ and U_{aa} is a unit matrix of order $a \times a$. Multiplication of the first matrix of Eq. (22) by α en-

ables us to write the matrix at the left-hand side of Eq. (27), after using Eq. (25), as $[\alpha\cdot Q + P(EB - A)P]^{-1}$. Furthermore, from Eqs. (25), (26), and (27) we get the following form of T_{bb} (the subscripts bb are eliminated):

$$T = P[\alpha\cdot Q + P(EB - A)P]^{-1}P. \tag{28}$$

We remark here also that $\partial T/\partial\alpha = 0$, i.e., T is independent of α.[27] Equations (23) and (28) show that T, Q, and P satisfy the relation

$$QT = TQ = 0. \tag{29a}$$

Additionally, giving the matrix $D = \alpha\cdot Q + P(EB - A)P$ and using the fact that $DD^{-1} = 1, PDD^{-1}P = P$, and Eq. (28), we obtain

$$P(EB - A)T = P. \tag{29b}$$

For the further development of the technique we define a matrix Ω by

$$\Omega = Q + T(A - EB)Q. \tag{30}$$

Multiplying this matrix from the left side by $P(A - EB)$ and using Eq. (29b), we get

$$\begin{aligned} P(A - EB)\Omega &= P(A - EB)Q + P(A - EB)T(A - EB)Q \\ &= P(A - EB)Q - P(A - EB)Q = 0, \end{aligned}$$

i.e.,

$$P(A - EB)\Omega = 0. \tag{31}$$

However, multiplication of Ω by $(A - EB)$ yields

$$\begin{aligned} (A - EB)\Omega &= (P + Q)(A - EB)\Omega = Q(A - EB)\Omega \\ &= Q(A - EB + (A - EB)T(A - EB))Q. \end{aligned} \tag{32}$$

Equation (32) indicates that the matrix Ω is an eigenmatrix of A, i.e., it satisfies the eigenvalue problem

$$A\Omega = EB\Omega, \tag{33}$$

if and only if

$$Q(A - EB + (A - EB)T(A - EB))Q = 0 \tag{34a}$$

is fulfilled. This leads to the relation

$$EQBQ = Q(A + (A - EB)T(A - EB))Q, \tag{34b}$$

which is exactly Eq. (11) in terms of the projection matrices Q and P.

The orthogonality conditions (14), however, can be expressed, using Eqs. (24c) and (24d), by

$$QBP = PBQ = 0. \tag{35}$$

Therefore from Eqs. (28) and (35) we conclude that

$$TBQ = QBT = 0 \tag{36}$$

holds and, accordingly, the matrix Ω shrinks to the form

$$\Omega = Q + TAQ. \tag{37}$$

Consequently, the equation corresponding to (12), with $QBQ = 1$, is given by

$$E = f(E) = Q(A + ATA)Q, \tag{38}$$

where the function $f(E)$ possesses the properties discussed in Sec. 2. Equation (38) also demands that the matrix Ω presented in Eq. (37) is an eigenmatrix of A. In connection with Eqs. (31) and (33), we remark that Ω given by Eq. (30) [or Eq. (37)] is a non-self-adjoint matrix satisfying the relations

$$Q\Omega = Q, \tag{39a}$$

$$\Omega Q = \Omega, \tag{39b}$$

and

$$P\Omega = \Omega - Q. \tag{39c}$$

4. GENERALIZED FORMALISM

In order to represent Eqs. (11), (12), (34b), and (38) in terms of operators in Hilbert space, we proceed by considering a reference-space $|\xi\rangle$, where $\langle\xi|\xi\rangle = 1$ holds. The associated projection operator Q is given by

$$Q = |\xi\rangle\langle\xi| \tag{40}$$

and its orthogonal complement P has the form

$$P = 1 - Q. \tag{41}$$

These operators also satisfy the relations

$$Q^+ = Q, \quad Q^2 = Q, \tag{42a}$$

$$P^+ = P, \quad P^2 = P, \tag{42b}$$

and

$$PQ = QP = 0. \tag{42c}$$

Analogous to Eq. (28), we define the "resolvent" operator

$$T = P[\alpha\cdot Q + P(EH_2 - H_1)P]^{-1}P, \tag{43}$$

where H_1 and H_2 are positive definite and Hermitian operators satisfying Eq. (2). The parameter α indicates a nonzero number and the relation $\partial T/\partial\alpha = 0$ specifies that T is independent of α. Consequently, it is easy to show that the relations

$$P(EH_2 - H_1)T = P \tag{44a}$$

and

$$QT = TQ = 0 \tag{44b}$$

are true. Moreover, we consider an operator Ω, such that

$$\Omega = Q + T(H_1 - EH_2)Q. \tag{45}$$

Operating on Eq. (45) from the left side by $P(H_1 - EH_2)$ we get, with the aid of Eq. (41a), the relation

$$P(H_1 - EH_2)\Omega = 0. \tag{46}$$

In the general case, however, we obtain

$$\begin{aligned} (H_1 - EH_2)\Omega &= (Q + P)(H_1 - EH_2)\Omega \\ &= Q(H_1 - EH_2)(1 + T(H_1 - EH_2))Q \\ &= Q(H_1 - EH_2 + (H_1 - EH_2) \\ &\quad \times T(H_1 - EH_2))Q. \end{aligned} \tag{47}$$

Therefore Ω is an eigenoperator of H_1, i.e.,

$$H_1\Omega = EH_2\Omega, \tag{48}$$

if and only if the equation

$$Q(H_1 - EH_2 + (H_1 - EH_2)T(H_1 - EH_2))Q = 0 \tag{49}$$

is fulfilled. This provides us with the formula

$$EQH_2Q = Q(H_1 + (H_1 - EH_2)T(H_1 - EH_2))Q, \tag{50}$$

which is similar to Eqs. (11) and (34a) [notice that the opera-

tor Ω also satisfies Eqs. (39a)–(39c)].

Let us now assume that the reference-space $|\xi\rangle$ is one dimensional and relates to another vector $|\phi\rangle$ by

$$Q|\phi\rangle = |\xi\rangle, \tag{51}$$

i.e.,

$$\langle\phi|Q|\phi\rangle = 1. \tag{52}$$

Moreover, let $|\psi\rangle$ be a vector defined by

$$\begin{aligned}|\psi\rangle = \Omega|\phi\rangle &= (Q + T(H_1 - EH_2)Q)|\phi\rangle \\ &= |\xi\rangle + T(H_1 - EH_2)|\xi\rangle.\end{aligned} \tag{53}$$

Operating with H_1 and using Eq. (48), we get

$$H_1|\psi\rangle = H_1\Omega|\phi\rangle = EH_2|\psi\rangle, \tag{54}$$

which is BGEP presented in Eq. (2). In other words the demand that Eq. (50) is true leads to a solution for BGEP. This solution is obtained by applying Ω on the vector $|\phi\rangle$ of Eq. (51). Additionally, an implicit relation for the energy E can be derived from (50) by multiplying from the right and left side by the vectors $|\phi\rangle$ and $\langle\phi|$, respectively. This leaves us with

$$E = \frac{\langle\xi|H_1 + (H_1 - EH_2)T(H_1 - EH_2)|\xi\rangle}{\langle\xi|H_2|\xi\rangle} \tag{55}$$

[note that Eq. (55) corresponds to Eq. (12) in the original formalism].

The orthogonality conditions (14) and (35) can be extended to the present case by requiring that

$$QH_2P = PH_2Q = 0 \tag{56}$$

holds. This is equivalent to choosing the reference-space $|\xi\rangle$ to be $|\xi\rangle = H_2^{1/2}|\xi\rangle$, where H_2 is positive definite, i.e., $H_2^{1/2}$ exists. Therefore, the normalization of this space is expressed by

$$\langle\xi|H_2|\xi\rangle = 1. \tag{57}$$

Substitution from Eq. (56) into Eq. (50) leads, with the help of Eq. (43), to the relation

$$EQH_2Q = Q(H_1 + H_1TH_1)Q, \tag{58}$$

where Q, P, and T are given by Eqs. (40), (41), and (43) after using the new form of $|\xi\rangle$. Also on operating (58) with the vector $|\phi\rangle$ and its complex conjugate we get, analogous to Eq. (55), the equality

$$E = f(E) = \frac{\langle\xi|H_1 + H_1TH_1|\xi\rangle}{\langle\xi|H_2|\xi\rangle}. \tag{59}$$

Also from Eqs. (43), (56), and (45), we obtain the reduced form of the operator Ω by

$$\Omega = Q + TH_1Q, \tag{60}$$

which satisfies Eq. (48) and operates on $|\phi\rangle$ projecting out the exact eigenvector $|\psi\rangle$ of BGEP. [Notice the similarity between Eqs. (59) and (60) and (37) and (30), respectively, presented in Ref. 27]. Having Eq. (57), it is easy to show that $f(E)$ has the following derivative:

$$\begin{aligned}f'(E) &= -\langle\xi|H_1T^2H_1|\xi\rangle \\ &= -\langle TH_1\xi|TH_1\xi\rangle < 0.\end{aligned} \tag{61}$$

Also defining a functional $F(E)$ by

$$F(E) = E - f(E) = 0, \tag{62a}$$

we conclude that

$$F'(E) = 1 - f'(E) > 0 \tag{62b}$$

holds. Thus the Newton–Raphson iteration procedure can be used for treating BGEP in an equivalent manner as the original approach of Löwdin and one can show that each successive value of E confines the exact eigenvalue.[30]

5. ENERGY-LOWER BOUNDS FOR BGEP

From the representations of the previous section we realize that the whole technique holds further, when the operator T [Eq. (43)] is replaced by a generalized one,

$$T = P(\alpha\cdot Q + P(\epsilon H_2 - H_1)P)^{-1}P, \tag{63}$$

where the parameter ϵ is an arbitrary (real or complex) variable. Moreover T satisfies the following relations:

$$P(\epsilon H_2 - H_1)T = P, \tag{64a}$$

$$QT = TQ = 0. \tag{64b}$$

Putting $P = 1 - Q$ into Eq. (64a) and using Eq. (56), we get

$$(\epsilon H_2 - H_1)T = 1 - Q(1 + H_1T). \tag{65}$$

[Equation (65) indicates that the reference-space (57) is employed]. We now assume that a vector $|\phi\rangle$ exists, such that

$$|\phi\rangle = TH_1|\xi\rangle \tag{66}$$

is valid. Applying the operator $(\epsilon H_2 - H_1)$ on $|\phi\rangle$ and using Eq. (40), we obtain

$$(\epsilon H_2 - H_1)|\phi\rangle = (H_1 - \langle\xi|H_1|\xi + \phi\rangle)|\xi\rangle. \tag{67}$$

Therefore, if $|\xi + \phi\rangle$ is replaced by a vector $|\psi_\epsilon\rangle$, Eq. (67) leads to the simple form

$$(\epsilon H_2 - H_1)|\psi_\epsilon\rangle = (\epsilon H_2 - \langle\xi|H_1 + H_1TH_1|\xi\rangle)|\xi\rangle. \tag{68}$$

This equation states that ϵ and $|\psi_\epsilon\rangle$ are the exact eigenvalue and eigenvector of BGEP, if and only if the functional

$$\epsilon_1 = f(\epsilon) = \frac{\langle\xi|H_1 + H_1TH_1|\xi\rangle}{\langle\xi|H_2|\xi\rangle} \tag{69}$$

is equivalent to ϵ. Thus the solution of BGEP is reduced to the calculation of the roots of the relation

$$F(\epsilon) = \epsilon - \epsilon_1 = 0. \tag{70}$$

The derivatives of the functionals $f(\epsilon)$ and $F(\epsilon)$ have the following properties:

$$f'(\epsilon) = -\langle\xi|H_1T^2H_1|\xi\rangle < 0 \tag{71}$$

and

$$F'(\epsilon) = 1 - f'(\epsilon) > 0. \tag{72}$$

The first inequality can be used, in addition to the Lagrange mean-value theorem,[31,37] to show that if $\Delta_1 = E - \epsilon$ and $\Delta_2 = E - \epsilon_1$ are the errors in ϵ and ϵ_1, respectively, with respect to the exact eigenvalue E, then Δ_1 and Δ_2 are always of different signs. This fact is known as the "bracketing theory" and leads to the important result that in case Δ_1 is selected to be negative (e.g., by choosing ϵ from Bubnov–Galerkin's variational method), then the corresponding Δ_2 must be positive and ϵ_1 is a lower bound to the exact energy

E. Thus we get the inequality

$$E > \epsilon_1 = \langle \xi | H_1 + H_1 P \frac{1}{\alpha \cdot Q + P(\epsilon_{up} H_2 - H_1)P} P H_1 | \xi \rangle, \tag{73}$$

where ϵ_{up} is an upper bound to E calculated from the relation

$$E < \epsilon_{up} = \frac{\langle \psi_t^{(n)} | H_1 | \psi_t^{(n)} \rangle}{\langle \psi_t^{(n)} | H_2 | \psi_t^{(n)} \rangle} = \text{minimum}. \tag{74}$$

The vector $|\psi_t^{(n)}\rangle$ of Eq. (74) is the superposition of the first n Hilbert-space vectors defined in Eq. (3). Finally, we notice that the lower bounds determined by (73) depend on the goodness of ϵ_{up} with respect to the exact value E. It is also clear that these lower bounds are applicable only for the first (lowest) eigenvalue of Eq. (2). Calculations of other bounds demand further arrangements, especially for the reference-space $|\xi\rangle$, of the technique.

6. DISCUSSION

The partitioning technique developed in Secs. 2–5 is actually a generalization of the original formulations of Löwdin.[27–32] It is obvious that these formulations correspond to the special case H_2 is a unitary operator. In fact the difficulty of treating BGEP has been removed in the above technique by introducing an adequate reference-space. This allows us to extend all properties of Löwdin's approach, in a straightforward manner, to the present formalism. Thus we can derive, for example, lower bounds for higher eigenvalues by proceeding similar to Löwdin[32] and Wilson[37] (see a forthcoming paper).

The advantage of the present technique, however, is that it can be applied to all cases where Schrödinger's equation (1) is converted into a BGEP with H_1 and H_2 Hermitian (not necessarily differential) operators.[39–43] In fact, it is also essential for the above technique that H_1 and H_2 are definite and H_2 is positive. However, if H_1 is positive and H_2 is known to be negative, then one can replace Eq. (2) by the conjugate (or reciprocal) eigenvalue problem[52,53]

$$H_2|\psi\rangle = \mu H_1 |\psi\rangle,$$

where $\mu = 1/E$, and proceed similarly to the above technique. In this case, the final form of the lower bounds will be given by (73) after changing H_1 by H_2 and vice versa.

ACKNOWLEDGMENTS

I should like to thank Professor J. S. Briggs for his generous help and interest in this work. I am also indebted to the group of atomic and molecular physics in Freiburg University. My thanks go to Frl. S. Ackermann for typing the manuscript.

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Construction of $(JJ^*)^{-1}$ in the Chandler–Gibson reaction theory [a)]

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(Received 20 January 1981; accepted for publication 24 July 1981)

We exhibit a technique to construct formally the operators $(JJ^*)^{-1}$ and $(JJIJ^*)^{-1}$ in the Chandler–Gibson theory. Our construction is based on integral equations whose kernels can be made contractive with an appropriate choice of parameters. We discuss uniqueness and give representations of the solutions as uniformly convergent series.

PACS numbers: 03.65.Ge

I. INTRODUCTION

The Chandler–Gibson equations[1,2] are unique among N-body reaction theories in many respects. Among the outstanding features are (i) the natural approximations have a very clean geometric content, (ii) the input involves only subsystem bound state wave functions and potentials, (iii) the equations only couple transition operators projected on channel subspaces, and (iv) the poles of the resolvent kernel of the integral equations are in 1-1 correspondence with the N-body binding energies. The structure of the equations and consequently the above properties arise naturally out of the two-Hilbert space setting[1-3] in which the time-dependent problem is cast. The second Hilbert space is the direct sum of the asymptotic channel spaces which is the space on which the scattering operator is expected to be unitary. At one level, this framework is just a notational device to make the multichannel multiparticle problem look something like a single-channel two-body problem. On the other hand, this framework respects the geometry of the problem to such an extent that the above features arise primarily as consequences of this choice of framework.

The two-Hilbert space approach of Chandler and Gibson has two other features that distinguish them from other N-body reaction theories. The first is that the kernel of the integral equations never becomes compact after any number of iterations, even though the solution of the equations is unique.[1,2] The other feature is the appearance of the operator $(JJ^*)^{-1}$ which has no analog in other N-body theories. Both of these properties require looking at the computational aspects of the scattering problem in a different light. Chandler and Gibson have shown that the theory of A-proper operators[4] can be applied, with a slight modification, to deal with the solution of the dynamical equations. This theory leads to a constructive method of solution of the Chandler–Gibson equations in the same sense that compact-kernel methods do for standard theories.

The operator $(JJ^*)^{-1}$ requires an additional calculation to construct the input to the dynamical equations. Chandler and Gibson have introduced an auxiliary operator M that can be constructed without the use of $(JJ^*)^{-1}$ and from which the exact transition operators can be obtained. The M equations are not as formally appealing as the transition operator equations in that they do not have unique solutions. In addition, the construction of the transition operators in terms of the M operator require the extraction of singular quantities. These considerations, along with present limited calculational experience,[5] indicates that approaching the problem directly in terms of the transition operator equations should not be hastily discarded. One practical reason for this is that a large fraction of the work required to construct $(JJ^*)^{-1}$ involves computing functions. These same functions have to be computed in order to construct the kernel of the M equations as well. Thus, this work is not avoided in either case, and the additional complications involved in computing $(JJ^*)^{-1}$ may be easier to deal with than difficulties that one is likely to encounter with the M-equation approach.

The purpose of this paper is to introduce techniques for constructing $(JJ^*)^{-1}$ in both the exact and approximate Chandler–Gibson equations. The method we consider provides an integral equation with a contractive kernel for the operators in question. This reduces the construction of $(JJ^*)^{-1}$ to uniformly convergent perturbation theory.

II. DEFINITIONS AND PROPERTIES OF $(JJ^*)^{-1}$

We being by assuming that we have an N-particle system whose infinitesimal time evolution is governed by a Hamiltonian, H. We denote partitions of this N-particle system into disjoint subsystems or clusters by lower case Latin letters $a, b, c, \cdots$. We use the notation n_a for the number of clusters of the partition a. To each partition a with $n_a > 1$, we associate the asymptotic configuration where the individual clusters of a are separated beyond the range of mutual interaction. In this region, the dynamics is well described by the partition Hamiltonian, H_a, which is obtained from H by turning off all interactions between particles in different clusters of a. Corresponding to each H_a is an invariant subspace, $\mathscr{M}_a$, which is the manifold of the N-particle Hilbert space spanned by the generalized eigenstates of H_a for which all particles in the same cluster of a are bound. For some configurations $\mathscr{M}_a$ may be empty. For the unique N-cluster partition $\mathbf{0}$, $\mathscr{M}_0$ is the entire N-body Hilbert space $\mathscr{H}$. For each a with $n_a > 1$, we let P_a denote the orthogonal projector on the subspace $\mathscr{M}_a$. For $a = \mathbf{0}$, we have $P_0 = 1$.

We introduce the following operators:

$$V^a \equiv H - H_a, \tag{2.1}$$

$$G_a(z) \equiv (z - H_a)^{-1}, \tag{2.2}$$

$$G(z) \equiv (z - H)^{-1}, \tag{2.3}$$

a)Work supported by the U. S. Department of Energy.

 0022-2488/81/122854-04$01.00

$$X \equiv JJ^* = \sum_a{}' P_a, \tag{2.4}$$

$$U^{ab}(z) \equiv V^b + V^a G(z) V^b, \tag{2.5}$$

$$T^{ab}(z) = P_a U^{ab}(z) P_b, \tag{2.6}$$

where in (2.4) and all that follows, we use the notation Σ'_a to denote $\Sigma_{\{a|n_a \neq 1\}}$. The Chandler–Gibson equations are equations for $T^{ab}(z)$ and have the form

$$T^{ab}(z) = P_a V^b P_b + \sum_c{}' P_a V^a X^{-1} P_c G_c(z) T^{cb}(z). \tag{2.7}$$

The natural approximations to this system of equations involve the replacements $P_a \to \Pi_a$, $X \to X_\Pi = \Sigma'_a \Pi_a$, where the Π_a's are assumed to satisfy

$$\text{(i) } \Pi_a = \Pi_a^2 = \Pi_a^*, \tag{2.8}$$

$$\text{(ii) } [\Pi_a, H_a]_- = 0, \tag{2.9}$$

$$\text{(iii) } X_\Pi = \sum_a{}' \Pi_a \text{ has a bounded inverse on the closure of its range.} \tag{2.10}$$

Most Π_a's of interest also satisfy $\Pi_a P_a = P_a \Pi_a = \Pi_a$, i.e., they project on a subspace of the corresponding $\mathscr{M}_a$. Also, in most approximations of interest, many of the Π_a's are zero. Our object is to provide equations for constructing X^{-1} and X_Π^{-1}.

III. TECHNICAL RESULTS

The equations that we ultimately construct result from certain assumptions on the operators under consideration. Although these assumptions have been verified elsewhere,[1] we include proofs here for completeness. The first result is due to Chandler and Gibson.[1,2]

Theorem 3.1: X has a bounded inverse, X^{-1}, that satisfies $\|X^{-1}\| \geqslant 1$.

Proof: Since $P_0 = 1$ we may express X in the form

$$X = 1 + \sum_{a \neq 0}{}' P_a. \tag{3.1}$$

X is clearly bounded, self-adjoint, and satisfies

$$(\psi, X\psi) = (\psi, \psi) + \sum_{a \neq 0}{}' (P_a\psi, P_a\psi),$$

$$= \|\psi\|^2 + \sum_{a \neq 0}{}' \|P_a\psi\|^2 \geqslant 0. \tag{3.2}$$

Equation (3.2) implies that the numerical range[6] of X is contained in the interval $[1, B_N - 1]$, where B_N is the Nth Bell number,[7] which is the number of partitions of N particles. Since the spectrum is a subset of the numerical range[6] we have $\sigma(X) \subseteq [1, B_N - 1]$, which immediately implies that X^{-1} exists and satisfies $\|X^{-1}\| \geqslant 1$.[8]

The second major result that we need concerns the specification of the ranges of sums of orthogonal projectors.

Theorem 3.2: Let $\{\Pi_a\}$ satisfy (2.8) and define X_π by

$$X_\pi = \sum_a{}' \Pi_a. \tag{3.3}$$

Then

$$\text{(i) } \overline{\mathscr{R}(X_\pi)} \supseteq \overline{\mathscr{R}(\Pi_a)} \tag{3.4}$$

and if (2.10) is also satisfied

$$\text{(ii) } \mathscr{R}(X_\pi) = \overline{\mathscr{R}(X_\pi)}, \tag{3.5}$$

where $\mathscr{R}(A)$ and $\overline{\mathscr{R}(A)}$ are the range and closure of the range of A, respectively.

Proof: Since X_π and Π_a are bounded self-adjoint operators we can express the Hilbert space $\mathscr{H}$ as a direct sum

$$\mathscr{H} = \mathscr{N}(X_\pi) \oplus \overline{\mathscr{R}(X_\pi)} \tag{3.6}$$

$$= \mathscr{N}(\Pi_a) \oplus \overline{\mathscr{R}(\Pi_a)}, \tag{3.7}$$

where $\mathscr{N}(A)$ is the null space of A. Since X_π and Π_a also satisfy $X_\pi \geqslant 0$ and $\Pi_a \geqslant 0$ the null spaces can be characterized by

$$\psi \in \mathscr{N}(X_\pi) \text{ iff } (\psi, X_\pi \psi) = 0, \tag{3.8}$$

$$\psi \in \mathscr{N}(\Pi_a) \text{ iff } (\psi, \Pi_a \psi) = 0. \tag{3.9}$$

But

$$(\psi, X_\pi \psi) = \sum_a{}' (\psi, \Pi_a \psi), \tag{3.10}$$

which requires that $\psi \in \mathscr{N}(X_\pi)$ implies $\psi \in \mathscr{N}(\Pi_a)$ or

$$\mathscr{N}(X_\pi) \subseteq \mathscr{N}(\Pi_a). \tag{3.11}$$

If we combine this result with the direct-sum decompositions above we obtain (i).

To show (ii), we let $\{\psi_n\} \in \mathscr{R}(X_\pi)$ with $\psi_n \to \psi$ and prove $\psi \in \mathscr{R}(X_\pi)$. Since X_π has a bounded inverse on $\overline{\mathscr{R}(X_\pi)}$, we can define the sequence $\{\phi_n\} \in \overline{\mathscr{R}(X_\pi)}$ by $\phi_n = X_\pi^{-1}\psi_n$ which represents the unique element in the inverse image of ψ_n under X_π in $\overline{\mathscr{R}(X_\pi)}$. Now clearly

$$\|\phi_m - \phi_n\| \leqslant \|X_\pi^{-1}\|_{\overline{\mathscr{R}(X_\pi)}} \|\psi_m - \psi_n\|, \tag{3.12}$$

where

$$\|X_\pi^{-1}\|_{\overline{\mathscr{R}(X_\pi)}} = \sup_{\substack{\|\psi\| = 1 \\ \psi \in \overline{\mathscr{R}(X)}}} \|X_\pi^{-1}\psi\|. \tag{3.13}$$

Since $\{\psi_n\}$ is convergent and $\|X_\pi^{-1}\|_{\overline{\mathscr{R}(X_\pi)}}$ is bounded, it follows that $\{\phi_n\}$ is Cauchy and converges to a unique $\phi \in \mathscr{H}$. Thus, since X_π is bounded

$$X_\pi \phi = \lim_{n \to \infty} X_\pi \phi_n = \lim_{n \to \infty} \psi_n = \psi,$$

which proves $\psi \in \mathscr{R}(X_\pi)$ and Eq. (3.4).

IV. INTEGRAL EQUATIONS

In this section, we write down integral equations for X^{-1} and X_π^{-1} and discuss some of their properties. We begin by considering X^{-1}. The most important point is that the spectrum of X is real, bounded above 0 and below ∞, as discussed in the proof of Theorem 3.1. This means that if we multiply X by a sufficiently small parameter $\alpha > 0$ we can rescale the spectrum to fall between 0 and 1. With such a choice, one expects

$$\|(1 - \alpha X)\| < 1. \tag{4.1}$$

The reason that this is of value is that through simple algebraic relations, we can obtain the equation

$$X^{-1} = \alpha + (1 - \alpha X) X^{-1}. \tag{4.2}$$

This equation has a unique solution for any $\alpha \neq 0$ by Theorem (3.1). If we find an α such that (4.1) is satisfied, then (4.2) has a contractive kernel and the sum

$$\sum_{n=0}^{\infty} (1 - \alpha X)^n \alpha \tag{4.3}$$

converges to X^{-1} in the uniform operator topology.

The required result is

Theorem 4.1: If $0 < \alpha < 2 \inf_{\|\psi\|=1} (\psi, X\psi)/\|X\|^2$, then (4.1) holds.

Proof: By definition (4.1) is equivalent to

$$\sup_{\|\psi\|=1} \{1 - 2\alpha(\psi, X\psi) + \alpha^2 \|X\psi\|^2\} < 1,$$

where we have used $X = X^*$ to obtain (3.3). This will clearly be satisfied provided

$$0 < \alpha < 2 \inf_{\|\psi\|=1} (\psi, X\psi) / \sup_{\|\psi\|=1} \|X\psi\|^2$$

$$= 2 \inf_{\|\psi\|=1} (\psi, X\psi)/\|X\|^2, \tag{4.4}$$

which is the desired condition.

It is easy to obtain weaker bounds that are somewhat more useful in practice.

Corollary 4.1: If $0 < \alpha < 2/\|X\|^2 \leqslant 2/(B_N - 1)^2$ then (4.1) holds. This follows immediately from (3.2) and (4.4).

Of greater interest is the construction of X_π^{-1}. This is trickier since X_π^{-1} exists uniquely only when it is considered as an operator on $\overline{\mathscr{R}(X_\pi)}$. What is actually needed in the dynamic equations is $X^{-1}{}_\pi H_a$, which makes sense by Theorem 3.2.

The equation corresponding to (4.2) for $X_\pi^{-1} H_a$ is

$$(X_\pi^{-1} H_a) = \alpha H_a + (1 - \alpha X_\pi) X_\pi^{-1} H_a, \tag{4.5}$$

which is easily obtained given (3.3) and

$$X_\pi X_\pi^{-1} = H_{\overline{\mathscr{R}(X_\pi)}}, \tag{4.6}$$

where $H_{\overline{\mathscr{R}(X_\pi)}}$ is the orthogonal projector on $\overline{\mathscr{R}(X_\pi)}$.

Given that X_π has a bounded inverse on $\mathscr{R}(X_\pi)$, $\|X_\pi\| < \infty$, $X_\pi \geqslant 0$, and $X_\pi = X_\pi^*$, one expects that one can find a sufficiently small α such that

$$\|(1 - \alpha X_\pi)\|_{\overline{\mathscr{R}(X_\pi)}} = \sup_{\substack{\|\psi\|=1 \\ \psi \in \mathscr{R}(X_\pi)}} \|(1 - \alpha X_\pi)\psi\| < 1. \tag{4.7}$$

Even though (4.5) does not have a unique solution on the N-body Hilbert space, if (4.7) holds, then the series

$$\sum_{m=1}^{\infty} (1 - \alpha X_\pi)^m \alpha H_a \tag{4.8}$$

converges to $X_\pi^{-1} H_a$ in the uniform operator topology since $(1 - \alpha X_\pi)$: $\overline{\mathscr{R}(X_\pi)} \to \overline{\mathscr{R}(X_\pi)}$ and $\overline{\mathscr{R}(X_\pi)} \supseteq \overline{\mathscr{R}(H_a)}$ by Theorem 3.2. The same manipulations leading to (4.1) can be used to obtain

$$0 < \alpha/2 < \inf_{\substack{\|\psi\|=1 \\ \psi \in \mathscr{R}(X_\pi)}} (\psi, X_\pi \psi) / \sup_{\substack{\|\psi\|=1 \\ \psi \in \mathscr{R}(X_\pi)}} \|X_\pi \psi\|^2 \tag{4.9}$$

as a sufficient condition for (4.7).

To obtain more useful conditions implying (4.7), we prove the following lower bound on the numerator of (4.9).

Lemma 4.1:

$$\inf_{\substack{\|\psi\|=1 \\ \psi \in \mathscr{R}(X_\pi)}} (\psi, X_\pi \psi) \geqslant 1/\|X_\pi^{-1}\|_{\overline{\mathscr{R}(X_\pi)}} \tag{4.10}$$

Proof: Since X_π is a bounded, non-negative, self-adjoint operator on the N-body Hilbert space, it uniquely induces a bounded, non-negative, self-adjoint operator on the closed subspace $\mathscr{R}(X_\pi)$ considered as a Hilbert space with the induced topology. By abuse of notation, we denote this operator by X_π. Since X_π has a bounded inverse, 0 is in the resolvent set of X_π. From the spectral theorem, to each $\psi \in \mathscr{R}(X_\pi)$ there is a positive measure $d\mu_\psi(\lambda)$ satisfying

$$(\psi, X_\pi \psi) = \int_{\sigma(X_\pi)} \lambda \, d\mu_\psi(\lambda) \tag{4.11}$$

and

$$(\psi, \psi) = \int_{\sigma(X_\pi)} d\mu_\psi(\lambda). \tag{4.12}$$

Since X_π is non-negative, the resolvent set of X_π is open and contains 0, it follows that

$$\lambda_0 = \inf_{\lambda \in \sigma(X_\pi)} \lambda > 0. \tag{4.13}$$

As a consequence of the stated conditions on the spectrum and the functional calculus[8]

$$1/\lambda_0 = \sup_{\lambda \in \sigma(X_\pi)} |1/\lambda| = \|X_\pi^{-1}\|.$$

By (4.11) and (4.12) and the positivity of $d\mu_\phi(\lambda)$, we obtain

$$(\phi, X_\pi \phi) \geqslant \lambda_0 (\phi, \phi) = \frac{1}{\|X_\pi^{-1}\|_{\mathscr{R}(X_\pi)}} (\phi, \phi)$$

for all $\phi \in \mathscr{R}(X_\pi)$. The bound (4.10) follows by taking infimums, proving the theorem

Lemma (4.1) allows us to obtain a sufficient bound of α.

Corollary 4.2: If

$$0 < \alpha < \frac{2}{\|X_\pi^{-1}\|_{\overline{\mathscr{R}(X_\pi)}} \|X_\pi\|^2} \leqslant \frac{2}{(B_N - 1)^2} \frac{1}{\|X_\pi^{-1}\|_{\overline{\mathscr{R}(X_\pi)}}}, \tag{4.14}$$

then (4.7) holds.

V. CONCLUSION

In this paper, we have considered the problem of constructing X^{-1} and X_π^{-1} for use in the Chandler–Gibson equations. The construction discussed exhibits X^{-1} as the unique solution of the integral equation (4.2). The equation depends on a fixed parameter α, although the solution and uniqueness considerations are independent of the choice of $\alpha \neq 0$. We have exhibited a nonempty set of values of this parameter for which the kernel becomes contractive. For these choices of the parameter, the solution can be represented as a uniformly convergent series (4.3).

For the approximate Chandler–Gibson equations, one requires the operator X_π^{-1} which exists uniquely only on $\overline{\mathscr{R}(X_\pi)}$. We have shown $\mathscr{R}(X_\pi) = \overline{\mathscr{R}(X_\pi)} \supseteq \overline{\mathscr{R}(H_a)}$ so $X_\pi^{-1} H_a$ exists on the full Hilbert space. This is the unique solution of (4.5) on $\mathscr{R}(X_\pi)$. This equation also depends on a

parameter such that for sufficiently small values of the parameter, this solution can be represented by a uniformly convergent series (4.8). Again, sufficient bounds on this parameter are computed for convergence of this series. Unfortunately, even the weakest bounds require an *a priori* knowledge of a lower bound for $\|X_\pi^{-1}\|_{\overline{\mathscr{R}(X_\pi)}}$.

We have made no attempt to consider the conditions on a set of projectors for which X_π^{-1} is bounded on the closure of the range X_π. This condition is necessary for the uniqueness and convergence conditions quoted in the last section. This is also among the restrictions imposed by Chandler and Gibson on approximation schemes.

The equations introduced here do not have compact kernels, like the Chandler–Gibson equations, but nevertheless have unique solutions. In addition, these solutions can be represented as uniformly convergent power series. We remark that it is also possible to construct X^{-1}, and under some circumstances, X_π^{-1}, using compact-kernel techniques of the type suggested in Ref. 9. We have not considered these methods in this paper.

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Faddeev's equations in differential form: Completeness of physical and spurious solutions and spectral properties

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(Received 20 March 1981; accepted for publication 30 July 1981)

Faddeev type equations are considered in differential form as eigenvalue equations for non-self-adjoint channel space (matrix) Hamiltonians H_F. For these equations in both the spatially confined and infinite systems, the nature of the spurious (nonphysical) solutions is obvious. Typically, these together with the physical solutions (given extra technical assumptions) generate a regular biorthogonal system for the channel space. This property may be used to provide an explicit functional calculus for the then real eigenvalue scalar spectral H_F, to show that $\pm i\mathsf{H}_F$ generate uniformly bounded C_0 semigroups and to simply relate H_F to self-adjoint Hamiltonian-like operators. These results extend to the four-channel Faddeev type equations where the breakup channel is included explicitly.

PACS numbers: 03.65.Nk

I. INTRODUCTION

The Faddeev-like equations will be discussed here within the more general framework of arrangement channel quantum mechanics (see Kouri, Levin, and Krüger[1]) for N-distinguishable particles. The channels are defined to be partitions of the particle labels into clusters (irrespective of the stability of these clusters). Let H be the N-particle Hamiltonian (with center of mass kinetic energy removed for spatially-infinite systems) acting on a Hilbert space $\mathscr{H}$. The most significant feature of the theory is the decomposition of H into channel components $H_{\alpha\beta}$ such that

$$\sum_{\alpha} H_{\alpha\beta} = H \text{ for all } \beta \tag{1.1}$$

and α, β belong to the subset of channels of interest (see Hoffman, Kouri and Top[2]). The matrix H with components $H_{\alpha\beta}$ is called the channel-space Hamiltonian. The Hamiltonian H may be decomposed into kinetic and potential energy parts as $H = T + V$. Similarly the α channel Hamiltonian H_α may be decomposed as $H_\alpha = T + V_\alpha$, where V_α is the sum of the interparticle potentials internal to the clusters of α (Kowalski[3]). The sum of residual interactions between particles in different clusters of α is denoted by $V^\alpha = V - V_\alpha$ so $H = H_\alpha + V^\alpha$ for all α. Typically H is not self-adjoint or even normal and for pairwise interactions is chosen so that $H_{\alpha\alpha} = H_\alpha$ for all α. For this class of decompositions we write

$$\mathsf{H} = \mathsf{H}_0 + \mathsf{V}, \tag{1.2}$$

where $[\mathsf{H}_0]_{\alpha\beta} = \delta_{\alpha\beta} H_\beta$ and V is off-diagonal. Furthermore, the potentials in V^α are distributed between $[\mathsf{V}]_{\beta\alpha}$ for different $\beta \neq \alpha$ so that the scattering equations corresponding to this choice of H have a kernel for which some iterate is "connected" (Kowalski,[3] Polyzou and Redish,[4] Evans[5]). The prescription (1.1) incorporates the Faddeev[6] equations, the Baer–Kouri–Levin–Tobocman (BKLT)[7] channel coupling decomposition and a transposed form of the Bencze–Redish–Sloan (BRS)[5,8–10] equations.

Let a vector in the channel space $\mathscr{C} = \oplus_\alpha \mathscr{H}$ on which H operates be denoted by Ψ with Hilbert space components $|\Psi_\alpha\rangle$. A class of equivalent norms on $\mathscr{C}$ may be induced naturally from the $\mathscr{H}$-norm.[5] The channel-space form of the time-independent Schrödinger equation may be written as

$$\mathsf{H}\Psi = \lambda \Psi. \tag{1.3}$$

It then follows from (1.1) that either[2]

$$\sum_\alpha |\Psi_\alpha\rangle \neq 0, \ (H - \lambda)\cdot\sum_\alpha |\Psi_\alpha\rangle = 0 \tag{1.4}$$

or

$$\sum_\alpha |\Psi_\alpha\rangle = 0. \tag{1.5}$$

The former are called physical solutions since $\Sigma_\alpha |\Psi_\alpha\rangle$ is a Hilbert space eigenfunction for H so $\lambda = E \in \mathbb{R}$. The latter are called spurious solutions. This characterization applies to both normalizable and wavelike solutions.

For a spatially-infinite system, the imbedding of N-particle bound-cluster H eigensolutions into normalizable physical H eigenvectors is not clear from general arguments. This must be verified explicitly for each H as will be done in the Faddeev case. Possibly complex eigenvalue normalizable spurious solutions may exist in general.[11–14] It has been demonstrated previously that no such solutions exist in the Faddeev case.[6] For general H, it is typically assumed that there exists a unique imbedding of all two-cluster H scattering solutions into wavelike physical H eigensolutions (if the corresponding α appears in the channel decomposition). A possibly nonunique imbedding of multicluster scattering solutions is also typically assumed. From these we may pick a subset in one-to-one correspondence with the H solutions to be kept as physical H solutions and replace the rest with real eigenvalue wavelike spurious solutions.[2,5] These are simply "numerically spurious" linear combinations, e.g., differences, of imbedded scattering solutions corresponding to the same H solution but with asymptotic part chosen in different channel components. Thus they do not have physical asymptotic boundary conditions. In the Faddeev case they will be

[a]Operated for the U.S. Department of Energy by Iowa State University under contract No. W-7405-eng-82. This research was supported by the Director for Energy Research, Office of Basic Energy Science, WPAS-01-03-01-2.

 0022-2488/81/122858-14$01.00

obtained directly and have simple plane wave structure.

Traditionally, the spatially-infinite Faddeev equations are regarded as having no spurious solutions. Implicit in this statement is the requirement that, in addition to (1.3) and (1.5) such solutions must satisfy the homogeneous form of Faddeev's integral equations. This result rules out normalizable spurious solutions, as indicated previously, but not the wavelike ones described above which satisfy an inhomogeneous form of the integral equations.

For the spatially confined case it is possible to show that the (point) spectrum of H is imbedded into the (point) spectrum of H. However, in general no simple imbedding procedure for H eigensolutions is available and little is known about spurious solutions. These solutions will be analyzed completely in the Faddeev case.

A question of primary interest for any arrangement-channel Hamiltonian is that of the completeness and basis properties of the physical and spurious solutions on the channel space. By completeness of a set of vectors which may be normalizable and/or unnormalizable, we mean that any vector in $\mathscr{C}$ can be approximated in norm as a possibly partly continuous linear combination of these vectors. Note that for nonorthogonal sets there exists a distinction between completeness and the basis property. The latter is stronger, requiring that any vector in $\mathscr{C}$ can be represented as a unique possibly partly continuous linear combination of basis vectors (convergence in norm implied). Certain natural requirements on the imbedding of physical solutions necessary and sufficient for these completeness and basis properties are detailed in Appendix A.

Should the basis property hold, then it is natural to develop a functional calculus for the (scalar spectral) operator H.[5] Since H is not self-adjoint or normal, it is necessary to obtain the biorthogonal dual eigenvectors separately. We denote a vector in the dual channel space $\mathscr{C}'$ by ζ' with components $\langle\zeta_\alpha|$ and its action on $\Psi\in\mathscr{C}$ by

$$(\zeta', \Psi) = \sum_\alpha \langle\zeta_\alpha|\Psi_\alpha\rangle. \tag{1.6}$$

The dual eigenvectors of H satisfy

$$(\zeta', H\Psi) = \lambda\,(\zeta', \Psi) \quad \text{for all } \Psi\in\text{dom}(H) \tag{1.7}$$

or

$$H'\zeta' = \lambda\,\zeta', \tag{1.8}$$

where H' denotes the (Banach space) dual of H. We shall make use of the general result that a biorthorgonal dual to the H eigenvector corresponding to a Hilbert space solution $|\Psi(E)\rangle$ is given by

$$\langle\zeta(E)_\alpha| = \langle\Psi(E)| \quad \text{for all } \alpha. \tag{1.9}$$

These ideas will be developed for the Faddeev equations. For a discussion of these and other results for general H operators, e.g., closedness, spectral theory, semigroup theory, ..., the reader is referred to previous work.[5]

Faddeev's equations in differential form with pairwise interactions are considered first for a spatially confined system in Sec. II. Here the spectrum is discrete.[5] The imbedding of H eigensolutions and existence of real eigenvalue spurious solutions are examined in detail here. Except where there is an "accidental" coincidence of physical and spurious eigenvalues resulting in the "loss" of a physical eigenvector, these solutions together are complete and, with an extra technical assumption, form a basis on $\mathscr{C}$. Thus the program outlined earlier may be implemented to first construct biorthogonal dual vectors and then a functional calculus for the real eigenvalue scalar spectral (*-self-adjoint) Faddeev Hamiltonian H_F. The structure and properties of H_F are further elucidated here.

In the third section, the analogous treatment is given for the spatially-infinite case where the weak (unnormalizable) scattering solutions must be considered. Here the real eigenvalue spurious solutions are all plane wavelike, as may be easily verified directly. These results are extended in a number of ways in the fourth section to allow for true three-body forces.

In the concluding section we remark on the cluster interpretation of the wave function components as previously elucidated by L'Huillier, Redish, and Tandy.[15] Some observations are made for the more general Faddeev-like equations of these authors. The role of the Faddeev example in clarifying the structure of more general H is discussed and particularly its application to the analysis of related Hamiltonians, e.g., the three-particle BKLT.

II. FADDEEV'S EQUATIONS FOR A SPATIALLY CONFINED SYSTEM

We consider a spatially confined system of three particles. The confinement may be achieved by the inclusion in the Hamiltonian of an external potential V_c which goes to $+\infty$ as any of the particles approach the (piecewise smooth) boundary ∂R of some region R. Alternatively, we may suppose that the Hilbert and channel-space wave functions are defined on the interior of a box and a periodic boundary condition is imposed at the walls. If the potentials have a range greater than the box size, then they are regarded as suitably treated. Many of the relevant mathematical concepts used to describe the structure of H_F (or H) are most conveniently introduced first here where the spectrum is discrete.[5] This type of problem is also important for applications to statistical mechanics of reactive systems where a convenient representation is first required for a confined system of a finite number of particles.[2,16] It will be clear from the following analysis that some aspects of the interpretation of the components of the physical channel-space eigenvectors will carry over from the spatially infinite case.[15,16]

First we exhibit a simple formula for the imbedding of H eigensolutions into physical H_F eigenvectors. A set of real eigenvalue spurious solutions providing a basis for $\mathscr{S}$ are obtained by inspection after rearranging the Faddeev equations. Together these are complete and, with an extra technical assumption, form a basis on $\mathscr{C}$ provided there is no "accidental" coincidence of eigenvalues of the full and noninteracting Hilbert space Hamiltonians. Exploiting the simple structure of the spurious solutions in this case, we may obtain explicit expressions for the biorthogonal spurious dual eigenvectors (as well as the physical ones). Also a functional calculus for the real eigenvalue scalar spectral (*-

self-adjoint) H_F is readily obtained which, in particular, allows the analysis of semigroup properties. The structure of H_F is further elucidated by exhibiting a self-adjoint Hamiltonian-like operator to which H_F is "equivalent."

The particles are labeled 1, 2, 3, and we assume that they interact through pairwise potentials. Following the usual convention, the interaction potential between particles i and j is labeled V_k where $k \neq i,j$ and k also labels the channel $(k)(ij)$. In differential form, the analog of Faddeev's equations (for the spatially confined region) have the form

$$\mathsf{H}_F\Psi = \lambda\Psi, \quad \text{with } \Psi = \begin{pmatrix} |\Psi_1\rangle \\ |\Psi_2\rangle \\ |\Psi_3\rangle \end{pmatrix}. \tag{2.1}$$

For a system confined by an external potential as described above, Ψ is defined on R and

$$\mathsf{H}_F = \mathsf{H}_e + \mathsf{V}_F \tag{2.2}$$

where H_e and V_F may be chosen as

$$\mathsf{H}_e = \begin{pmatrix} T+V_e+V_1 & 0 & 0 \\ 0 & T+V_e+V_2 & 0 \\ 0 & 0 & T+V_e+V_3 \end{pmatrix}$$

and

$$\mathsf{V}_F = \begin{pmatrix} 0 & V_1 & V_1 \\ V_2 & 0 & V_2 \\ V_3 & V_3 & 0 \end{pmatrix}. \tag{2.3}$$

Implicitly the $\Psi|_{\partial R} = \mathbf{0}$.

For the periodic problem, Ψ is defined on the interior of a box with periodic boundary conditions imposed at the walls and

$$\mathsf{H}_F = \mathsf{H}_0 + \mathsf{V}_F, \tag{2.4}$$

where

$$\mathsf{H}_0 = \begin{pmatrix} T+V_1 & 0 & 0 \\ 0 & T+V_2 & 0 \\ 0 & 0 & T+V_3 \end{pmatrix}, \tag{2.5}$$

and with V_F defined as above. In both these cases T is the total kinetic energy of the three particles. The periodic problem has some special features reminiscent of an infinite system. In contrast to a system with a confining external potential, the center of mass kinetic energy operator may be naturally separated from the rest of the Hilbert or channel-space Hamiltonian resulting in a separation of variables factorization of the eigenfunctions. One part is a plane wave in the center of mass variable and provides a discrete center of mass kinetic energy contribution to the total energy. The other depends on the internal (e.g., Jacobi) variables and provides a discrete contribution from the relative motion to the total energy. Another feature of the periodic problem reminiscent of an infinite system is that the states involving a true bound cluster of all particle, should they exist, are "dynamically disconnected" from the states involving smaller clusters, e.g., in the three-particle periodic system the true three-particle bound clusters never dissociate into one- or two-particle clusters and are never formed from these. Again this property is not true if we introduce an external wall potential.

The analysis of the channel-space equations for both spatially confined problems is similar so we present in detail here only the case with a confining external potential. In integral equation form, essentially the only difference between these two cases occurs in the various Green's functions through the eigenfunctions providing their spectral representation. Since with an external potential, the boundary conditions on the wave functions are made explicit by incorporating the external potential in the Green's functions, this case is notationally more convenient to consider. Here $H = T + V_e + \Sigma_{k=1}^3 V_k$ and the corresponding Hilbert space Schrödinger equation

$$H|\Psi\rangle = E|\Psi\rangle \quad (|\Psi\rangle|_{\partial R} = 0) \tag{2.6}$$

has a complete orthonormal set of solutions, $|\Psi(n)\rangle$, in $\mathscr{H}$ which are labeled by an index n and have discrete real eigenvalues E_n.

Let us suppose first that none of the E_n "accidently" coincides with the eigenvalues of the noninteracting Hamiltonian $H_e = T + V_e$. Now consider the imbedding of solutions (2.6) into the solution set of the corresponding Faddeev equations (2.1). It is clear that $|\Psi(n)\rangle$ must satisfy the homogeneous integral equation

$$|\Psi(n)\rangle = G_e(E_n)V|\Psi(n)\rangle, \tag{2.7}$$

where $V = \Sigma_{i=1}^3 V_i$ and $G_e(z) = (z - H_e)^{-1}$. There is, of course, no inhomogeneous term since $E_n - H_e$ is invertible. The corresponding channel-space vector $\Psi(n)$ is defined to have components

$$|\Psi_j(n)\rangle = G_e(E_n)V_j|\Psi(n)\rangle \quad j = 1, 2, 3, \tag{2.8}$$

(cf. L'Huillier *et al.*[15]). It will be assumed here the potentials are such that $|\Psi_j(n)\rangle$ is normalizable for all n, e.g., H_e-bounded will do. From (2.7), it is a trivial matter to show that $\Psi(n)$ satisfies the differential equation

$$\mathsf{H}_F\Psi(n) = E_n\Psi(n) \tag{2.9}$$

and the homogeneous integral equation

$$\Psi(n) = \mathsf{G}_e(E_n)\mathsf{V}_F\Psi(n), \tag{2.10}$$

with $\mathsf{G}_e(z) = (z - \mathsf{H}_e)^{-1}$ provided E_n is not an eigenvalue of H_e. Otherwise a modified inhomogeneous integral equation for $\Psi(n)$ must be constructed.

Next we consider the spurious solutions. It is convenient to rewrite the Faddeev equations (2.1) in the form

$$(\lambda - (T + V_e))|\Psi_k\rangle = V_k\Big(\sum_{j=1}^{3}|\Psi_j\rangle\Big), \quad k = 1, 2, 3. \tag{2.11}$$

By definition the right-hand side of each equation is identically zero for the spurious solutions. Let us denote a complete orthonormal set of solutions of

$$H_e|\Psi\rangle = (T + V_e)|\Psi\rangle = \lambda|\Psi\rangle \quad (|\Psi\rangle|_{\partial R} = 0) \tag{2.12}$$

by $|\phi(n)\rangle$ where $\lambda = E_n^0$ is the corresponding real eigenvalue. For certain simple choices of V_e, we can write them down explicitly. (e.g., if V_e corresponds to a box, then the $|\phi(n)\rangle$ are given in terms of sinusoidal functions.) A set of spurious solutions forming a basis on $\mathscr{S} = \{\Psi \in \mathscr{C} : \Sigma_{j=1}^3 |\Psi_j\rangle = 0\}$

can now be chosen as $\{\phi^1(n), \phi^2(n)\}$ where

$$\phi^i(n) = \theta^i|\phi(n)\rangle \quad i = 1, 2, \tag{2.13}$$

where $\theta^i = (\theta^i_1, \theta^i_2, \theta^i_3)^T$, $i = 1, 2$ are linearly independent numerical spurious vectors, i.e., $\Sigma^3_{j=1}\theta^i_j = 0$, $i = 1, 2$.

These spurious solutions satisfy the differential equation

$$\mathsf{H}_F\phi^i(n) = E^0_n\phi^i(n) \quad i = 1, 2, \tag{2.14}$$

and the homogeneous integral equation

$$\phi^i(n) = \mathsf{G}_e(E^0_n)\mathsf{V}_F\phi^i(n) \quad i = 1, 2, \tag{2.15}$$

provided E^0_n is not an eigenvalue of H_e. Otherwise a modified inhomogeneous integral equation for $\phi^i(n)$ must be constructed.

Since all the physical solutions are imbedded in $\mathscr{C}$ and $\{\phi^1(n), \phi^2(n)\}$ span $\mathscr{S}$, it follows from the discussion of Appendix A that $\{\Psi(n), \phi^1(n), \phi^2(n)\}$ are complete on $\mathscr{C}$, i.e., any vector in $\mathscr{C}$ can be approximated arbitrarily closely by finite linear combinations of these.

Next we consider the biorthogonal dual eigenvectors of H_F which satisfy

$$\mathsf{H}'_F\zeta' = \lambda\,\zeta'. \tag{2.16}$$

A discussion of this equation has been given by Sandhas.[17] The solutions $\zeta'(n)$ of (2.16) corresponding to the $\Psi(n)$ are characterized by having all components equal (cf. Sec. I), i.e.,

$$(\zeta'(n))_j = \sum_{k=1}^{3}\langle\Psi_k(n)| = \langle\Psi(n)|, \quad \text{for all } j. \tag{2.17}$$

Then

$$\mathsf{H}'_F\zeta'(n) = E_n\zeta'(n). \tag{2.18}$$

the $\phi^i(n)$, $\Psi(m)$ and $\zeta'(n)$ satisfy the biorthogonal relationships[2,5,18–20]

$$\begin{aligned}(\zeta'(n), \Psi(m)) &= \delta_{m,n},\\ (\zeta'(n), \phi^i(m)) &= 0.\end{aligned} \tag{2.19}$$

We aim to complete this biorthogonal system by constructing vectors $\zeta^{i'}(n)$, $i = 1, 2$, which are dual vectors to the spurious solutions, satisfying

$$\begin{aligned}(\zeta^{i'}(n), \Psi(m)) &= 0,\\ (\zeta^{i'}(n), \phi^j(m)) &= \delta_{m,n}\delta_{i,j}.\end{aligned} \tag{2.20}$$

If we assume that for some class of potentials, all l^2 linear combinations of $\Psi(n)$ converge in norm (l^2 assumption), then $\{\Psi(n), \phi^1(n), \phi^2(n)\}$ form a basis for $\mathscr{C}$ in addition to being complete.[21] Furthermore the $\zeta^{i'}(m)$ are uniquely prescribed by (2.20) and it is easily verified that[5]

$$\mathsf{H}'_F\zeta^{i'}(m) = E^0_m\zeta^{i'}(m). \tag{2.21}$$

The set $\{\zeta'(n), \zeta^{1'}(n), \zeta^{2'}(n)\}$ is called the associated sequence of coefficient functionals[19] for $\{\Psi(n), \phi^1(n), \phi^2(n)\}$. We shall not investigate here the range of validity of the l^2 assumption. Note however that the l^2 convergence is certainly always true for the sum of the components. From the Hahn–Banach theorem,[22] the existence and uniqueness of the $\zeta^{i'}(n)$ follows if each $\phi^i(n)$ is a finite distance from the span of the other eigenvectors. The need here is to guarantee the separation of the closure of the span of the $\Psi(n)$ from nonzero vectors in $\mathscr{S}$.

These results may be expressed succinctly as:

Theorem 1: Under the l^2 assumption, the set $\{\zeta'(n), \zeta^{1'}(n), \zeta^{2'}(n); \Psi(n), \phi^1(n), \phi^2(n)\}$ is a regular biorthogonal system for $\mathscr{C}$ providing a resolution of the identity

$$1 = \sum_n\Psi(n)\zeta'(n) + \sum_{i=1}^{2}\sum_n\phi^i(n)\zeta^{i'}(n). \tag{2.22}$$

Furthermore, the sum over any subset of terms in (2.22) gives a bounded (non-self-adjoint) projection operator onto an H_F-invariant subspace of $\mathscr{C}$.

Proof: Equation (2.22) follows from the previous discussion, as does the projection operator property. We remark that boundedness for finite sums is obvious and boundedness for any subset of terms is proved by taking an approximating sequence of finite sums and using the Banach–Steinhaus theorm.[22] □

From Theorem 1, in particular, the projection operators

$$\mathsf{P} = \sum_n\Psi(n)\zeta'(n), \quad \left(\mathsf{Q} = \sum_{i=1}^{2}\sum_n\phi^i(n)\zeta^{i'}(n)\right) \tag{2.23}$$

for the physical (spurious) solutions are bounded. We now use these facts to give an explicit construction of the dual eigenvectors $\zeta^{i'}(n)$ corresponding to the spurious solutions. Pick θ^3 to be any vector such that $\Sigma^3_{j=1}\theta^3_j \neq 0$, θ^i $i = 1, 2$ as previously. Let $\{\theta^1, \theta^2, \theta^3; \chi^{1\prime}, \chi^{1\prime\prime}, \chi^{3\prime}\}$ be a complete biorthogonal system in $\mathbb{R}^3$, then $\chi^{3\prime} = c(1, 1, 1)$. Next define dual vectors

$$\hat{\zeta}^{i'}(n) = \langle\phi(n)|\chi^{i'} \quad i = 1, 2, \tag{2.24}$$

then

$$(\hat{\zeta}^{i'}(n), \phi^j(m)) = \delta_{i,j}\delta_{n,m} \quad i, j = 1, 2 \tag{2.25}$$

so

$$\begin{aligned}\zeta^{i'}(n) &= \hat{\zeta}^{i'}(n)\mathsf{Q}\\ &= \hat{\zeta}^{i'}(n) - \hat{\zeta}^{i'}(n)\mathsf{P}\\ &= \hat{\zeta}^{i'}(n) - \sum_m(\hat{\zeta}^{i'}(n), \Psi(m))\zeta'(m).\end{aligned} \tag{2.26}$$

The right-hand side is given in terms of known vectors and the sum converges since P is bounded.

The structure of H_F is described by

Theorem 2: Under the l^2 assumption, a countably additive resolution of the identity (spectral family) for H_F is given by

$$\mathsf{E}(\delta) = \sum_{E_n\in\delta}\Psi(n)\zeta'(n) + \sum_{i=1}^{2}\sum_{E^0_n\in\delta}\phi^i(n)\zeta^{i'}(n), \tag{2.27}$$

where δ are Borel sets in the complex plane; (here, on the real line would suffice). Thus H_F is a spectral operator.[5] Furthermore

$$\begin{aligned}\mathsf{H}_F\Psi &= \sum_n E_n(\zeta'(n), \Psi)\Psi(n)\\ &\quad + \sum_{i=1}^{2}\sum_n E^0_n(\zeta^{i'}(n), \Psi)\phi^i(n)\\ &= \int_{\Delta(\mathsf{H}_F)}\lambda\,\mathsf{E}(d\lambda)\Psi,\end{aligned} \tag{2.28}$$

where $\Psi \in \mathrm{dom}(\mathsf{H}_F)$ and $\Delta(\mathsf{H}_F)$ is an open set containing the spectrum of H_F. Thus H_F is also scalar spectral.[5,23]

Proof: These results have been discussed previously for general H.[5] We remark that the proof of the scalar spectral property uses that H_F is closed for potentials of interest. □

The difference between the spectral and scalar spectral properties for an arbitrary operator is described in Appendix B. As a corollary of Theorem 2, we have that H_F is *-self-adjoint where the involution * is associated with the conjugate linear duality mapping D: $\mathscr{C} \to \mathscr{C}'$ given by

$$D\Psi(n) = \zeta'(n), \quad D\phi^i(n) = \zeta^{i'}(n), \tag{2.29}$$

i.e.,

$$(D\Psi, \mathsf{H}_F\phi) = (D\mathsf{H}_F\Psi, \phi), \quad \forall \Psi, \phi \in \mathscr{C}. \tag{2.30}$$

For general channel-space Hamiltonians H, *-self-adjointness can only be guaranteed for the restrictions of H to the H-invariant subspace spanned by the physical eigenvectors.[5]

A functional calculus may now be defined for H_F (loosely) by

$$f(\mathsf{H}_F) = \int_{\Delta(\mathsf{H}_F)} f(\lambda)\mathsf{E}(d\lambda), \tag{2.31}$$

or more explicitly by

$$f(\mathsf{H}_F) = \sum_n f(E_n)\Psi(n)\zeta'(n) + \sum_{i=1}^{2}\sum_n f(E_n^0)\phi^i(n)\zeta^{i'}(n); \tag{2.32}$$

(cf. the functional calculus for normal or self-adjoint operators). A form of the functional calculus involving a contour integral is also available.[24] It is easy to see that boundedness of $f(\ )$ ensures convergence of the sums from (2.32) for $f(\mathsf{H}_F)\Psi$ for any $\Psi \in \mathscr{C}$ since

$$\sum_n f(E_n)\Psi(n)(\zeta'(n), \Psi) = \sum_n f(E_n)\Big(\Psi(n)\Big|\sum_\alpha [\Psi]_\alpha\Big)\Psi(n), \tag{2.33}$$

which is an l^2 linear combination of the $\Psi(n)$ and,

$$\sum_{i=1}^{2}\sum_n f(E_n^0)\phi^i(n)(\zeta^{i'}(n), \Psi) = \sum_{i=1}^{2}\sum_n f(E_n^0)(\hat{\zeta}^{i'}(n), (1-\mathsf{P})\Psi)\phi^i(n), \tag{2.34}$$

which is an l^2 linear combination of plane waves in each component since $(\hat{\zeta}^{i'}(n), (1-\mathsf{P})\Psi)$ is a linear combination of Fourier coefficients of the components of $(1-\mathsf{P})\Psi$.[21] This vector is in $\mathscr{C}$ since P is bounded. Furthermore, applying the Banach–Steinhaus theorem, we see that $f(\ )$ is bounded ensures that $f(\mathsf{H}_F)$ is bounded.

This property is particularly important for the time-dependent theory where operators of the form $e^{\pm i/\hbar \mathsf{H}_F t}$ are of interest. Let us examine in more detail here the properties of these semigroups. The following preliminary result is useful:

Lemma 3: Let J: $\mathscr{H} \to \mathscr{C}$ be the injection operator for the physical solutions so

$$J|\Psi(n)\rangle = \Psi(n) \quad \text{for all } n. \tag{2.35}$$

Then under the l^2 assumption J is bounded so if $|\Psi\rangle = \Sigma_n f_n|\Psi(n)\rangle$ then

$$\|\Psi\|_{\mathscr{C}} \leq |||J|||\cdot\|\Psi\|_{\mathscr{H}} = |||J|||\Big(\sum_n |f_n|^2\Big)^{1/2} \quad \text{where } |||J||| < +\infty \tag{2.36}$$

Proof: Boundedness follows from that of P since $J = \mathsf{P}\theta$ where $\Sigma_{i=1}^3(\theta)_i = 1$. A direct proof may also be given using the Banach–Steinhaus theorem. As a simple consequence of the lemma and Eqs. (2.32)–(2.34), we now have

Theorem 3: Under the l^2 assumption, $\pm i\mathsf{H}_F$ are the infinitesimal generators of uniformly bounded C_0 semigroups[25] $e^{\pm i/\hbar \mathsf{H}_F t}$.

We remark that the existence for general H with strictly bounded potentials of $e^{\pm i/\hbar \mathsf{H} t}$ has been demonstrated.[5,26] These will not in general be uniformly bounded.

Clearly there is a similarity between the structure of the Faddeev Hamiltonian H_F and a self-adjoint Hamiltonian-type operator. This is further elucidated by the following result:

Theorem 4: Under the l^2-assumption, H_F is equivalent to the self-adjoint operator

$$\begin{pmatrix} H & 0 & 0 \\ 0 & H_e & 0 \\ 0 & 0 & H_e \end{pmatrix}$$

in the sense that there exists a bounded invertible operator B_F such that

$$\mathsf{B}_F\mathsf{H}_F\mathsf{B}_F^{-1} = \begin{pmatrix} H & 0 & 0 \\ 0 & H_e & 0 \\ 0 & 0 & H_e \end{pmatrix}. \tag{2.37}$$

Proof: By direct construction. A complete set of orthogonal eigenvectors for this self-adjoint operator may be chosen as

$$\Psi_0(n) = \begin{pmatrix} |\Psi(n)\rangle \\ 0 \\ 0 \end{pmatrix}, \quad \phi_0^1(n) = \begin{pmatrix} 0 \\ |\phi(n)\rangle \\ 0 \end{pmatrix}, \quad \phi_0^2(n) = \begin{pmatrix} 0 \\ 0 \\ |\phi(n)\rangle \end{pmatrix}. \tag{2.38}$$

The corresponding orthogonal dual vectors are denoted by $\zeta_0'(n)$, $\zeta_0^{1'}(n)$, $\zeta_0^{2'}(n)$. The operator B_F is given by

$$\mathsf{B}_F = \sum_n \Psi_0(n)\zeta'(n) + \sum_{i=1}^{2}\sum_n \phi_0^i(n)\zeta^{i'}(n). \tag{2.39}$$

Boundedness, as usual, follows from the l^2 assumption and the Banach–Steinhaus theorem. From orthogonality and biothogonality,

$$\mathsf{B}_F^{-1} = \sum_n \Psi(n)\zeta_0'(n) + \sum_{i=1}^{2}\sum_n \phi^i(n)\zeta_0^{i'}(n). \quad \square \tag{2.40}$$

This equivalence further clarifies the way the physics is imbedded into Faddeev's Hamiltonian (as well as the appearance of spurious solutions). A corresponding equivalence

property holds for general scalar spectral operators H where $\pm iH$ generate uniformly bounded semigroups.[23] As a corollary to the theorem, we have that

$$\mathsf{B}_F(\mathsf{H}_F\mathsf{P})\mathsf{B}_F^{-1} = \begin{pmatrix} H & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{2.41}$$

We remark that the duality mapping D with respect to which H_F is *-self-adjoint is related to B_F by

$$D = C\mathsf{B}_F^{*}\mathsf{B}_F \tag{2.42}$$

Here C: $\mathscr{C} \to \mathscr{C}'$ is the usual Hilbert space conjugate linear isomorphism. Also observe that Theorem 4 may be used as an alternative basis for providing a functional calculus of H_F leading simply to such results as Theorem 3.

Finally we note that throughout this section we have assumed that none of the eigenvalues of H and H_c "accidentally" coincide. Should this happen, it is possible to lose the corresponding physical eigenvector which is "replaced" by a spurious one. The scalar spectral property of the Faddeev Hamiltonian then no longer holds. This case is discussed in detail in Appendix C.

III. FADDEEV'S EQUATIONS FOR A SPATIALLY INFINITE SYSTEM

These equations are obtained from (2.1)–(2.3) by removing the external wall potential and adopting the resulting equations for Ψ defined everywhere, i.e.,

$$\mathsf{H}_F\Psi = \lambda\Psi, \quad \text{where } \mathsf{H}_F = \mathsf{H}_0 + \mathsf{V}_F, \tag{3.1}$$

with H_0 and V_F defined as previously. In the spatially-infinite case it is convenient to assume that the center-of-mass kinetic energy has been removed from T.

We first exhibit a simple imbedding formula for the true three-particle bound states as well as the asymptotic two-cluster scattering solutions. For the breakup channel (asymptotic three-cluster) scattering solutions, a somewhat more complicated formula is derived from formal manipulation of the corresponding integral equations. A set of real eigenvalue plane wave spurious solutions providing a basis for $\mathscr{S}$, the real eigenvalue scalar spectral (*-self-adjoint) property, functional calculus and semigroup properties of H_F as well as equivalence to a self-adjoint Hamiltonian-like operator are easily demonstrated as in the previous section.

The Hilbert space Hamiltonian H for this system is assumed to have a complete set of eigenvectors (including the "weak" scattering solutions). Let $|\Psi(n)\rangle$ denote the normalized true three-body bound states and $|\Psi_\alpha^{\pm}(\mathbf{k}^\alpha, m)\rangle$, $\alpha = 1, 2, 3$, denote the scattering solutions for channel α where particle α scatters off a bound state of the other particles (if such bound states exist). The wave vector $\mathbf{k}^\alpha$ describes the relative asymptotic momentum of particle α and the bound state; m is the quantum number for the associated two-particle bound state; the total energy (excluding center-of-mass energy) is denoted by $E = E(\mathbf{k}^\alpha, m)$. The breakup-channel scattering solutions where the three particles are asymptotically free are denoted by $|\Psi_0^{\pm}(\mathbf{k}^0)\rangle$. Here $\mathbf{k}^0$ denotes the suitably chosen pair of wave vectors for the relative asymptotic momenta with a corresponding kinetic energy $E = E(\mathbf{k}^0)$ (excluding center-of-mass energy). These wave vectors can most conveniently be given as a pair of relative Jacobi momenta. $+(-)$ denotes a pre- (post-) collisional choice of these asymptotic conditions. Completeness of H implies that

$$1 = \sum_n |\Psi(n)\rangle\langle\Psi(n)| + \sum_{\alpha=0}^{3}\sum_m \int d\mathbf{k}^\alpha |\Psi_\alpha^{\pm}(\mathbf{k}^\alpha, m)\rangle\langle\Psi_\alpha^{\pm}(\mathbf{k}^\alpha, m)|. \tag{3.2}$$

Certain of these solutions may be imbedded directly into channel-space solutions following a procedure analogous to that of the last section.

The true three-particle bound state solutions satisfy

$$|\Psi(n)\rangle = G_0(E_n)V|\Psi(n)\rangle, \tag{3.3}$$

where $G_0(z) = (z - T)^{-1}$ and provided $E_n < 0$. If $E_n > 0$, then $G_0(E_n)$ (or $G_0(E_n)V$) is regarded as having been suitably regularized. We define a channel-space vector $\Psi(n)$ with components

$$|\Psi_j(n)\rangle = G_0(E_n)V_j|\Psi(n)\rangle, \quad j = 1, 2, 3, \tag{3.4}$$

and if $E_n > 0$, the regularization of $G_0(E_n)$ is chosen so that the r.h.s. lies in $\mathscr{H}$. This vector satisfies $\Sigma_{j=1}^3 |\Psi_j(n)\rangle = |\Psi(n)\rangle$ and

$$\mathsf{H}_F\Psi(n) = E_n\Psi(n). \tag{3.5}$$

If E_n is not in the (continuous) spectrum $C\sigma(\mathsf{H}_0)$ of H_0 (i.e., of $H_j = T + V_j$ for any j),[27] then $\Psi(n)$ satisfies the homogeneous integral equation

$$\Psi(n) = \mathsf{G}_0(E_n)\mathsf{V}_F\Psi(n), \tag{3.6}$$

where $\mathsf{G}_0(z) = (z - \mathsf{H}_0)^{-1}$. If $E_n \in C\sigma(\mathsf{H}_0)$, then $\mathsf{G}_0(E_n)$ is regarded as suitably regularized.

The asymptotic two-cluster ($\alpha = 1, 2, 3$) scattering solutions also satisfy

$$|\Psi_\alpha^{\pm}(\mathbf{k}^\alpha, m)\rangle = G_0^{\pm}(E)V|\Psi_\alpha^{\pm}(\mathbf{k}^\alpha, m)\rangle \quad \alpha = 1, 2, 3, \tag{3.7}$$

where $E = E(\mathbf{k}^\alpha, m)$ and $G_0^{\pm}(E) = \lim_{\epsilon\to 0} G_0(E \pm i\epsilon)$ ($= G_0(E)$ if $E < 0$). We define channel-space vectors $\Psi_\alpha^{\pm}(\mathbf{k}^\alpha, m)$, $\alpha = 1, 2, 3$, with components

$$|\Psi_{\alpha j}^{\pm}(\mathbf{k}^\alpha, m)\rangle = G_0^{\pm}(E)V_j|\Psi_\alpha^{\pm}(\mathbf{k}^\alpha, m)\rangle, \quad j = 1, 2, 3 \tag{3.8}$$

so this vector satisfies $\Sigma_{j=1}^3 |\Psi_{\alpha j}^{\pm}(\mathbf{k}^\alpha, m)\rangle = |\Psi_\alpha^{\pm}(\mathbf{k}^\alpha, m)\rangle$ and

$$\mathsf{H}_F\Psi_\alpha^{\pm}(\mathbf{k}^\alpha, m) = E\Psi_\alpha^{\pm}(\mathbf{k}^\alpha, m), \tag{3.9}$$

or in integral form,

$$\Psi_\alpha^{\pm}(\mathbf{k}^\alpha, m) = \phi_\alpha(\mathbf{k}^\alpha, m) + \mathsf{G}_0^{\pm}(E)\mathsf{V}_F\Psi_\alpha^{\pm}(\mathbf{k}^\alpha, m), \tag{3.10}$$

where $(\phi_\alpha(\mathbf{k}^\alpha, m))_j = \delta_{\alpha j}|\phi(\mathbf{k}^\alpha)\rangle \otimes |\phi_m\rangle$. $|\phi(\mathbf{k}^\alpha)\rangle$ is a plane wave for particle α of relative momentum $\mathbf{k}^\alpha$ and $|\phi_m\rangle$ and is the mth bound state solution of the appropriate two-particle problem. Also $\mathsf{G}_0^{\pm}(E) = \lim_{\epsilon\to 0}\mathsf{G}_0(E \pm i\epsilon)$. It is assumed here that the potentials are such that the $\Psi(n)$ are in $\mathscr{C}$ (H_0-bounded will do) and the $\Psi_\alpha^{\pm}(\mathbf{k}^\alpha, m)$ are suitably well-behaved.[27]

For the breakup-channel (asymptotic three-cluster)

scattering solutions, the above imbedding procedure is not applicable. However, a somewhat more complicated imbedding formula is derived below by resuming the formal solution of the appropriate channel-space integral equation. First denote by $|\phi_j^{\pm}(\mathbf{k}^0)\rangle$ the two-particle scattering solutions of the equation $(T+V_j-E)|\phi\rangle=0$ with asymptotic wave number $\mathbf{k}^0$. The wave function $|\phi_j^{\pm}\rangle$ factors as a product of a plane wave for particle j and a two-particle scattering solution for the other particles. If we define two-particle T matrices by $t_j^{\pm}=V_j+V_jG_0^{\pm}t_j^{\pm}$ then $G_j^{\pm}V_j=G_0^{\pm}t_j^{\pm}$, $V_jG_j^{\pm}=t_j^{\pm}G_0^{\pm}$, $V_j|\phi_j^{\pm}\rangle=t_j^{\pm}|\phi\rangle$, and $|\phi_j^{\pm}\rangle$ $=(1+G_0^{\pm}t_j^{\pm})|\phi\rangle$, where $|\phi\rangle$ is the corresponding three-particle plane wave. The breakup-channel solution $\Psi_0^{\pm}$ may be chosen as any of $\Psi_{0(j^*)}^{\pm}$, $j^*=1,2,3$, satisfying the integral equation

$$\Psi_{0(j^*)}^{\pm}(\mathbf{k}^0)=\phi_{0(j^*)}^{\pm}(\mathbf{k}^0)+G_0^{\pm}(E)V_F\Psi_{0(j^*)}^{\pm}(\mathbf{k}^0), \tag{3.11}$$

where $E=E(\mathbf{k}^0)$ and $(\phi_{0(j^*)}^{\pm})_k=\delta_{kj^*}|\phi_{j^*}^{\pm}\rangle$. Formal expansion of the solution yields

$$(\Psi_{0(j^*)}^{\pm})_k=\delta_{kj^*}|\phi\rangle+G_0^{\pm}t_k^{\pm}|\phi\rangle+G_0^{\pm}t_k^{\pm}\times\Big(\sum_{j\neq k}G_0^{\pm}t_j^{\pm}+\sum_{j\neq k}G_0^{\pm}t_j^{\pm}\sum_{l\neq j}G_0^{\pm}t_l^{\pm}+\cdots\Big)\Big|\phi\Big\rangle. \tag{3.12}$$

However, since $|\Psi_0^{\pm}\rangle=|\phi_j^{\pm}\rangle+G_j^{\pm}V^j|\Psi_0^{\pm}\rangle$, we have that

$$\begin{aligned}&\sum_{j\neq k}G_0^{\pm}V_j|\Psi_0^{\pm}\rangle\\&=\sum_{j\neq k}(G_0^{\pm}V_j|\phi_j^{\pm}\rangle+G_0^{\pm}V_jG_j^{\pm}V^j|\Psi_0^{\pm}\rangle)\\&=\sum_{j\neq k}G_0^{\pm}t_j^{\pm}|\phi\rangle+\sum_{j\neq k}G_0^{\pm}t_j^{\pm}\sum_{l\neq j}G_0^{\pm}V_l|\Psi_0^{\pm}\rangle\\&=\cdots\\&=\Big(\sum_{j\neq k}G_0^{\pm}t_j^{\pm}+\sum_{j\neq k}G_0^{\pm}t_j^{\pm}\sum_{l\neq j}G_0^{\pm}t_l^{\pm}+\cdots\Big)|\phi\rangle.\end{aligned} \tag{3.13}$$

Consequently one obtains the imbedding formula

$$\begin{aligned}(\Psi_{0(j^*)}^{\pm})_k&=\delta_{kj^*}|\phi\rangle+G_0^{\pm}t_k^{\pm}|\phi\rangle\\&\quad+G_0^{\pm}t_k^{\pm}G_0^{\pm}\sum_{j\neq k}V_j|\Psi_0^{\pm}\rangle\\&=\delta_{kj^*}|\phi\rangle+G_0^{\pm}V_k|\phi_k^{\pm}\rangle\\&\quad+G_0^{\pm}V_kG_k^{\pm}\sum_{j\neq k}V_j|\Psi_0^{\pm}\rangle\quad k=1,2,3,\end{aligned} \tag{3.14}$$

which agrees with the result of Benoist-Gueutal and L'Huillier.[28] We may verify directly that $\Psi_{0(j^*)}^{\pm}$ defined by (3.14) satisfies (3.1).

Thus we have shown that the set $\{\Psi_{0(j^*)}^{\pm},\Psi_\alpha^{\pm},\alpha=1,2,3,\Psi(n)\}$, for each choice of j^*, is in one-to-one correspondence with the (physical) eigenvectors of the corresponding Hilbert space Hamiltonian.

The spurious solutions are most easily found by writing Faddeev's equations in a form analogous to (2.11) (for this case there is no external potential of course). Let $|\phi(\mathbf{k})\rangle$ be a complete set of solutions to

$$T|\phi(\mathbf{k})\rangle=E|\phi(\mathbf{k})\rangle, \tag{3.15}$$

labeled by a suitable wave vector $\mathbf{k}$. Then a set of spurious solutions $\{\phi^1(\mathbf{k}),\phi^2(\mathbf{k})\}$ providing a basis for $\mathscr{S}$ is given by

$$\phi^i(\mathbf{k})=\theta^i|\phi(\mathbf{k})\rangle\quad i=1,2, \tag{3.16}$$

where θ^i are defined as in the previous section.

Suppose that for a class of potentials, all L^2-linear combinations of the $\Psi_\alpha^{\pm}$ and $\Psi_0^{\pm}$ are convergent in norm and that such linear combinations where the energy is restricted to a Borel set of the real line form a closed subspace (L^2 assumption). This is of course true for the sum of the components and also for the individual components in asymptotic regions. (We shall not, however, investigate here the range of validity of the L^2 assumption.) It then follows from the discussion in Appendix A that $\{\Psi_{0(j^*)}^{\pm},\Psi_\alpha^{\pm},\alpha=1,2,3,\Psi(n)\}$ for each choice of j^* and $+$ or $-$, together with the spurious solutions $\{\phi^1,\phi^2\}$ form a basis for $\mathscr{C}$. Note that a suitable "limit-in-mean" interpretation will be required for the integrals representing linear combinations of these solutions (see Titchmarsh[29] for a discussion of this problem in the standard L^2–Fourier theory and Amrein *et al.*[30] for a more general case). As discussed previously[5] in a general context, the nonuniqueness of the choice of $\Psi_0^{\pm}$ guarantees the existence of spurious wavelike solutions with unphysical asymptotic boundary conditions. Indeed we could generate the set of spurious solutions described above by taking

$$\phi^i(k)=\sum_{j^*=1}^{3}\theta_{j^*}^i\Psi_{0(j^*)}^{\pm}(\mathbf{k})\quad i=1,2, \tag{3.17}$$

where from (3.14), each component of the r.h.s. is a plane wave as required. The integral equations for $\phi^i(\mathbf{k})$ now follow automatically from (3.11). Thus another choice of basis for $\mathscr{C}$ would be $\{\Psi_{0(j^*)}^{\pm},j^*=1,2,3,\Psi_\alpha^{\pm},\alpha=1,2,3,\Psi(n)\}$ (under the L^2 assumption) choosing either $+$ or $-$.

All the wavelike solutions discussed above do not lie in the channel space $\mathscr{C}$ and are thus termed more correctly "weak eigenvectors". They can be regarded as elements of a larger space $\mathscr{C}'$ dual to $\mathscr{C}$ where $\mathscr{C}\subset\mathscr{C}\subset\mathscr{C}'$ and $\mathscr{C}$ may be chosen as a Banach or countably-normed space dense in $\mathscr{C}$. The domain of H_F can be extended in $\mathscr{C}'$ to include wavelike functions.[5]

As in the spatially-confined case, it is useful to construct the dual vectors (associated sequence of coefficient functionals) corresponding to the chosen basis $\{\Psi(n);\Psi_\alpha,\alpha=0,1,2,3;\phi^i,i=1,2,\}$ for $\mathscr{C}$ (where from now on, we assume that some specific choice of j^* for $\Psi_0^{\pm}=\Psi_{0(j^*)}^{\pm}$ and of $+$ or $-$ has been made). They may be used to form a generalized biorthogonal system. The $\zeta'(n)$ and $\zeta'_\alpha(\mathbf{k}^\alpha,m)$ are given by

$$(\zeta'(n))_j=\sum_{k=1}^{3}\langle\Psi_k(n)|=\langle\Psi(n)|\quad\text{for all } j, \tag{3.18}$$

$$(\zeta'(\mathbf{k}^\alpha,m))_j=\Sigma_{k=1}^{3}\langle\Psi_{\alpha k}(\mathbf{k}^\alpha,m)|=\langle\Psi_\alpha(\mathbf{k}^\alpha,m)|\text{ for all } j,\ \alpha=0,1,2,3,$$

and they satisfy

$$\begin{aligned}&H_F'\zeta'(n)=E_n\zeta'(n),\\&H_F'\zeta'_\alpha(\mathbf{k}^\alpha,m)=E(\mathbf{k}^\alpha,m)\zeta'_\alpha(\mathbf{k}^\alpha,m)\quad\alpha=1,2,3,\\&H_F'\zeta'_0(\mathbf{k}^0)=E(\mathbf{k}^0)\zeta'_0(\mathbf{k}^0).\end{aligned} \tag{3.19}$$

The following generalized biorthogonal relationships are

also satisfied:

$$
\begin{aligned}
&(\zeta'(n), \Psi(m)) = \delta_{m,n},\\
&(\zeta'(n), \phi^i(\mathbf{k})) = (\zeta'(n), \Psi_\alpha(\mathbf{k}^\alpha, m)) = 0,\\
&(\zeta'_\alpha(\mathbf{k}^\alpha, m), \Psi_\beta(\mathbf{k}'^\beta, n)) = \delta_{\alpha,\beta}\delta_{m,n}\delta(\mathbf{k}^\alpha - \mathbf{k}'^\beta),\\
&(\zeta'_\alpha(\mathbf{k}^\alpha, m), \Psi(m)) = (\zeta'_\alpha(\mathbf{k}^\alpha, m), \phi^i(\mathbf{k})) = 0,\\
&\text{for } \alpha, \beta = 0, 1, 2, 3; \quad i = 1, 2.
\end{aligned}
\tag{3.20}
$$

The generalized biorthogonal system is completed by constructing dual vectors $\zeta^{i'}(\mathbf{k})$ to the spurious solutions, which satisfy

$$
\begin{aligned}
&(\zeta^{i'}(\mathbf{k}), \phi^j(\mathbf{k}')) = \delta_{i,j}\delta(\mathbf{k} - \mathbf{k}'),\\
&(\zeta^{i'}(\mathbf{k}), \Psi(n)) = (\zeta^{i'}(\mathbf{k}), \Psi_\alpha(\mathbf{k}^\alpha, m)) = 0.
\end{aligned}
\tag{3.21}
$$

Under the L^2 assumption, the above prescription of the $\zeta^{i'}(\mathbf{k})$ is unique in an almost everywhere sense and furthermore they satisfy

$$
\mathsf{H}'_F\zeta^{i'}(\mathbf{k}) = E(\mathbf{k})\zeta^{i'}(\mathbf{k}). \tag{3.22}
$$

Theorem 5: Under the L^2 assumption, the set

$$
\{\zeta'(n), \zeta'_0(\mathbf{k}), \zeta'_\alpha(\mathbf{k}^\alpha, m), \zeta^{i'}(\mathbf{k}'); \Psi(n), \Psi_0(\mathbf{k}), \Psi_\alpha(\mathbf{k}^\alpha, m), \phi^i(\mathbf{k}') \quad (\alpha = 1, 2, 3, \quad i = 1, 2)\}
$$

is a generalized regular biorthogonal system of $\mathscr{C}$ providing a resolution of the identity

$$
1 = \sum_n \Psi(n)\zeta'(n) + \sum_{\alpha=0}^{3}\sum_m \int d\mathbf{k}^\alpha\, \Psi_\alpha(\mathbf{k}^\alpha, m)\zeta'_\alpha(\mathbf{k}^\alpha, m) + \sum_{i=1}^{2}\int d\mathbf{k}\phi^i(\mathbf{k})\zeta^{i'}(\mathbf{k}). \tag{3.23}
$$

Furthermore if the sums and/or integrals in (3.23) are replaced by partial sums and/or integrals over Borel subsets, a bounded (non-self-adjoint) projection operator onto a H_F-invariant subspace of $\mathscr{C}$ results.

Proof: Formally, the proof is the same as for Theorem 1. Boundedness follows from the closure part of the L^2 assumption. From the countable additivity, it follows that this boundedness is uniform.[23] □

Explicit forms for the bounded projection operators onto the physical and spurious solutions are again available. The structure of H_F is described by

Theorem 6: Under the L^2 assumption, a countably additive resolution of the identity (spectral family) for H_F is given by

$$
\begin{aligned}
\mathsf{E}(\delta) = &\sum_{E_n\in\delta} \Psi(n)\zeta'(n)\\
&+ \sum_{\alpha=0}^{3}\sum_m \int_{E(\mathbf{k}^\alpha, m)\in\delta} d\mathbf{k}^\alpha\, \Psi_\alpha(\mathbf{k}^\alpha, m)\zeta'_\alpha(\mathbf{k}^\alpha, m)\\
&+ \sum_{i=1}^{2}\int_{E(\mathbf{k})\in\delta} d\mathbf{k}\,\phi^i(\mathbf{k})\zeta^{i'}(\mathbf{k}),
\end{aligned}
\tag{3.24}
$$

where δ are Borel sets in the complex plane; (here, in the real line would suffice). Thus H_F is a spectral operator. Furthermore,

$$
\begin{aligned}
\mathsf{H}_F\Psi &= \sum_n E_n(\zeta'(n), \Psi)\Psi(n)\\
&\quad + \sum_{\alpha=0}^{3}\sum_m \int d\mathbf{k}^\alpha\, E(\mathbf{k}^\alpha, m)(\zeta'_\alpha(\mathbf{k}^\alpha, m), \Psi)\Psi_\alpha(\mathbf{k}^\alpha, m)\\
&\quad + \sum_{i=1}^{2}\int d\mathbf{k}\, E(\mathbf{k})(\zeta^{i'}(\mathbf{k}), \Psi)\phi^i(\mathbf{k})\\
&= \int_{\Delta(\mathsf{H}_F)} \lambda \mathsf{E}(d\lambda)\,\Psi,
\end{aligned}
\tag{3.25}
$$

where $\Psi\in\mathrm{dom}(\mathsf{H}_F)$ and $\Delta(\mathsf{H}_F)$ is an open set containing the spectrum of H_F. Thus H_F is also scalar spectral.

Proof: Formally, the proof is the same as for Theorem 2. □

As a corollary of Theorem 6, we have that H_F is *-self-adjoint where the involution * is associated with the duality mapping induced by the regular biorthogonal system of eigenvectors (cf. Sec. II). A functional calculus may now be defined for H_F (loosely) by [cf. (2.31) and (2.32)]

$$
f(\mathsf{H}_F) = \int_{\Delta(\mathsf{H}_F)} f(\lambda)\,\mathsf{E}(d\lambda), \tag{3.26}
$$

or more explicitly by

$$
\begin{aligned}
f(\mathsf{H}_F) = &\sum_n f(E_n)\Psi(n)\zeta'(n)\\
&+ \sum_{\alpha=0}^{3}\sum_m \int d\mathbf{k}^\alpha f(E(\mathbf{k}^\alpha, m))\Psi_\alpha(\mathbf{k}^\alpha, m)\zeta'_\alpha(\mathbf{k}^\alpha, m)\\
&+ \sum_{i=1}^{2}\int d\mathbf{k}\, f(E(\mathbf{k}))\phi^i(\mathbf{k})\zeta^{i'}(\mathbf{k}).
\end{aligned}
\tag{3.27}
$$

The analogs of Theorems 3 and 4 hold for the spatially-infinite case. Thus, under the L^2 assumption, $\pm i\mathsf{H}_F$ generate uniformly bounded C_0 semigroups. In Appendix D, we describe the use of this result to obtain a prescription for the imbedding of normalized Hilbert space eigenfunctions via a mean ergodic theorem for H_F. Also H_F is equivalent to the self-adjoint operator

$$
\begin{pmatrix} H & 0 & 0\\ 0 & H_0 & 0\\ 0 & 0 & H_0 \end{pmatrix}
$$

in the sense that

$$
\mathsf{B}_F\mathsf{H}_F\mathsf{B}_F^{-1} = \begin{pmatrix} H & 0 & 0\\ 0 & H_0 & 0\\ 0 & 0 & H_0 \end{pmatrix}, \tag{3.28}
$$

where B_F is a bounded invertible operator which has a representation analogous to (2.39) and is simply related to the duality mapping with respect to which H_F is *-self-adjoint [cf. (2.42)].

An explicit construction of the dual vectors associated with the spurious solutions is a little more complicated here. Formally, the construction is the same as in the last section. If $\Psi_{0(j^*)}(\mathbf{k})$ is chosen as the physical breakup-channel solution, then pick θ^3 so that $\theta^3_i = \delta_{i,j^*}$ $i = 1, 2, 3$ and θ^1, θ^2 as previously. The corresponding biorthogonal duals satisfy $\chi^{3'} = (1, 1, 1)$ and $\chi^{i'}_{j^*} = 0$ for $i = 1, 2$. By analogy with (2.26)

we have

$$\xi^{i'}(\mathbf{k}) = \hat{\xi}^{i'}(\mathbf{k}) - \sum_n (\hat{\xi}^{i'}(\mathbf{k}), \Psi(n))\xi'(n) - \sum_{\alpha=0}^{3} \sum_m \int d\,\mathbf{k}^\alpha\, (\hat{\xi}^{i'}(\mathbf{k}), \Psi_\alpha(\mathbf{k}^\alpha, m))\xi'_\alpha(\mathbf{k}^\alpha, m), \quad (3.29)$$

where $\hat{\xi}^{i'}(\mathbf{k}) = \chi^{i'}\langle\phi(\mathbf{k})|$ with $\chi^{i'}$ described above. The inner product $(\hat{\xi}^{i'}(\mathbf{k}), \Psi(n))$ may be evaluated immediately as it is a convergent integral (at least as a "limit-in-mean"); however, the expression $(\hat{\xi}^{i'}(\mathbf{k}), \Psi_\alpha(\mathbf{k}^\alpha, m))$ may be regarded as a singular measure with respect to the wave vectors and must be considered more carefully (see Appendix E). Note that the $\chi^{i'}$ determine the asymptotic plane wave structure of the $\xi^{i'}(\mathbf{k})$ $(i = 1, 2)$ and $\xi'_0(\mathbf{k}^0)$ $(i = 3)$ as well as the inhomogeneous terms in the integral equations for these wave functions[5] (see Appendix F).

IV. FADDEEV'S EQUATIONS WITH A TRUE THREE-BODY POTENTIAL

In previous sections we have considered only the case of pairwise interactions between the three particles. Here we also allow for the possibility of a true three-body interaction V_{123} so the Hamiltonian of the system is given by $H = T + V_e + V_{123} + \Sigma_{k=1}^3 V_k$. In this work we shall consider only the spatially infinite case with $V_e \equiv 0$. An analysis of the simpler spatially confined problem analogous to Sec. II could easily be developed. The potential V_{123} may be introduced into the matrix Hamiltonian of Sec. III in many ways which satisfy the summation property (1.1). Those preserving a simple imbedding procedure are described below.

Consider the case where the potential V_{123} is introduced along any one of the three rows as, for example, in

$$H_F = \begin{pmatrix} T + V_1 + V_{123} & V_1 + V_{123} & V_1 + V_{123} \\ V_2 & T + V_2 & V_2 \\ V_3 & V_3 & T + V_3 \end{pmatrix}. \quad (4.1)$$

It is convenient to introduce some further notation. Let $V_{j+123} = V_j + V_{123}$, $H_{j+123} = T + V_{j+123}$, $G_{j+123}(z) = (z - H_{j+123})^{-1}$, and let $\phi^{\pm}_{j+123}$ satisfy $(E - H_{j+123})|\phi^{\pm}_{j+123}\rangle = 0$ and correspond asymptotically to a plane wave. Further define $t^{\pm}_{j+123} = V_{j+123} + V_{j+123} G_0^{\pm} t^{\pm}_{j+123}$ so $G^{\pm}_{j+123} V_{j+123} = G_0^{\pm} t^{\pm}_{j+123}$, $V_{j+123}|\phi^{\pm}_{j+123}\rangle = t^{\pm}_{j+123}|\phi\rangle$ and $|\phi^{\pm}_{j+123}\rangle = (1 + G_0^{\pm} t^{\pm}_{j+123})|\phi\rangle$.

The imbedding formulas for both the true three-particle bound states as well as the asymptotic two-cluster scattering solutions have the same form

$$|\Psi_1(n)\rangle = G_0(E_n)V_{1+123}|\Psi(n)\rangle,$$
$$|\Psi_j(n)\rangle = G_0(E_n)V_j|\Psi(n)\rangle, \quad j = 2, 3, \quad (4.2)$$

where suitable regularization is required if $E_n \geqslant 0$ and for $\alpha = 1, 2, 3$,

$$|\Psi^{\pm}_{\alpha 1}\rangle = G_0^{\pm}(E)V_{1+123}|\Psi^{\pm}_{\alpha}\rangle,$$
$$|\Psi^{\pm}_{\alpha j}\rangle = G_0^{\pm}(E)V_j|\Psi^{\pm}_{\alpha}\rangle \quad j = 2, 3. \quad (4.3)$$

An imbedding formula for the breakup-channel scattering solution may again be obtained from a formal resummation of the corresponding integral equation giving

$$(\Psi^{\pm}_{0\hat{0}^*})_1 = \delta_{1,j^*}|\phi\rangle + G_0^{\pm} t^{\pm}_{1+123}|\phi\rangle + G_0^{\pm} t^{\pm}_{1+123} G_0^{\pm}(V_2 + V_3)|\Psi^{\pm}_0\rangle,$$
$$(\Psi^{\pm}_{0\hat{0}^*})_k = \delta_{k,j^*}|\phi\rangle + G_0^{\pm} t^{\pm}_k|\phi\rangle + G_0^{\pm} t^{\pm}_k G_0^{\pm}(V_{1+123} + V_{\hat{k}})|\Psi^{\pm}_0\rangle, \quad \{k, \hat{k}\} = \{2, 3\}. \quad (4.4)$$

As should be clear from (4.4), the spurious solutions have exactly the same plane wave form as for the operator of Sec. III. Given an appropriate L^2 assumption, the results of that section on the real eigenvalue scalar spectral (*-self-adjoint) property, the semigroup property and equivalence to the self-adjoint Hamiltonian-like operator of (3.28) are again valid here.

Next we consider the case where the potential V_{123} is introduced along the diagonal

$$H_F = \begin{pmatrix} T + V_1 + V_{123} & V_1 & V_1 \\ V_2 & T + V_2 + V_{123} & V_2 \\ V_3 & V_3 & T + V_3 + V_{123} \end{pmatrix}. \quad (4.5)$$

Denote $H_{123} = T + V_{123}$, $G_{123}(z) = (z - H_{123})^{-1}$, and let $|\phi^{\pm}_{123}\rangle$ satisfy $(E - H_{123})|\phi^{\pm}_{123}\rangle = 0$ and correspond asymptotically to a plane wave. Further define $t^{\pm}_{j/123} = V_j + V_j G^{\pm}_{123} t^{\pm}_{j/123}$ so $G^{\pm}_{j+123} V_j = G^{\pm}_{123} t^{\pm}_{j/123}$, $V_j|\phi^{\pm}_{j+123}\rangle = t^{\pm}_{j/123}|\phi^{\pm}_{123}\rangle$ and $|\phi^{\pm}_{j+123}\rangle = (1 + G^{\pm}_{123} t^{\pm}_{j/123})|\phi^{\pm}_{123}\rangle$.

Let us suppose first that there is no eigenvalue common to the point spectra of H and H_{123} should these sets be nonempty. Then the imbedding formula for the true three-particle bound states is given by

$$|\Psi_j(n)\rangle = G_{123}(E_n)V_j|\Psi(n)\rangle, \quad j = 1, 2, 3, \quad (4.6)$$

where suitable regularization is required if $E_n \in C\sigma(H_{123}) = [0, \infty)$. Similarly, for the two-cluster scattering solutions $\alpha = 1, 2, 3$,

$$|\Psi^{\pm}_{\alpha j}\rangle = G^{\pm}_{123}(E)V_j|\Psi^{\pm}_{\alpha}\rangle, \quad j = 1, 2, 3. \quad (4.7)$$

From the same approach as described previously, one obtains for the breakup-channel solutions

$$(\Psi^{\pm}_{0\hat{0}^*})_k = \delta_{k,j^*}|\phi^{\pm}_{123}\rangle + G^{\pm}_{123} t^{\pm}_{k/123}|\phi^{\pm}_{123}\rangle + G^{\pm}_{123} t^{\pm}_{k/123} G^{\pm}_{123} \sum_{j\neq k} V_j|\Psi^{\pm}_0\rangle, \quad k = 1, 2, 3. \quad (4.8)$$

A set of spurious solutions providing a basis for $\mathscr{S}$ is given here by $\phi^i = \theta^i|\phi\rangle$, $i = 1, 2$ where $|\phi\rangle$ satisfies

$$(E - H_{123})|\phi\rangle = 0. \quad (4.9)$$

So as well as the spurious wavelike solutions apparent from (4.8), there may also be real-eigenvalue-normalizable spurious solutions. Under an appropriate L^2 assumption, the spectral and semigroup properties described previously again hold for this operator, except that it is now equivalent

to

$$\begin{pmatrix} H & 0 & 0 \\ 0 & H_{123} & 0 \\ 0 & 0 & H_{123} \end{pmatrix}.$$

Let us return to the case where there is an accidental coincidence of one or more eigenvalues of H and H_{123}. It is clear that the simple imbedding procedure for the bound-state solutions of H is no longer valid. If such a solution is missing then a simple adaptation of the discussion of Appendix C shows that a generalized eigenvector may be constructed instead as a replacement. The operator H_F under the L^2 assumption is type-one spectral.

A slightly different approach is to explicitly introduce a fourth breakup channel, still preserving the summation property (1.1). We consider (cf. Newton[31])

$$\mathsf{H}_F = \begin{pmatrix} T+V_{123} & V_{123} & V_{123} & V_{123} \\ V_1 & T+V_1 & V_1 & V_1 \\ V_2 & V_2 & T+V_2 & V_2 \\ V_3 & V_3 & V_3 & T+V_3 \end{pmatrix}, \tag{4.10}$$

which acts on vectors Ψ with four components $|\Psi_j\rangle, j=0,1,2,3$. The imbedding formulas for both the true three-particle bound states as well as the asymptotic two-cluster scattering solutions again have the same form

$$\begin{aligned} |\Psi_0(n)\rangle &= G_0(E_n)V_{123}|\Psi(n)\rangle, \\ |\Psi_j(n)\rangle &= G_0(E_n)V_j|\Psi(n)\rangle, \\ & \qquad j=1,2,3, \end{aligned} \tag{4.11}$$

where a suitable regularization is required if $E_n \geqslant 0$, and for $\alpha = 1, 2, 3$,

$$\begin{aligned} |\Psi^{\pm}_{\alpha 0}\rangle &= G_0^{\pm}(E)V_{123}|\Psi^{\pm}_{\alpha}\rangle, \\ |\Psi^{\pm}_{\alpha j}\rangle &= G_0^{\pm}(E)V_j|\Psi^{\pm}_{\alpha}\rangle, \\ & \qquad j=1,2,3. \end{aligned} \tag{4.12}$$

The usual approach for the breakup-channel solutions yields for $j^* = 0, 1, 2, 3$

$$\begin{aligned} (\Psi^{\pm}_{0(j^*)})_0 &= \delta_{0,j^*}|\phi\rangle \\ &\quad + G_0^{\pm}t^{\pm}_{123}|\phi\rangle + G_0^{\pm}t^{\pm}_{123}G_0^{\pm}\sum_{j=1}^{3}V_j|\Psi_0^{\pm}\rangle, \\ (\Psi^{\pm}_{0(j^*)})_k &= \delta_{0,j^*}|\phi\rangle \\ &\quad + G_0^{\pm}t_k^{\pm}|\phi\rangle + G_0^{\pm}t_k^{\pm}G_0^{\pm} \\ &\quad \times\Big(V_{123}+\sum_{j\neq k}V_j\Big)|\Psi_0^{\pm}\rangle, \\ & \qquad k=1,2,3, \end{aligned} \tag{4.13}$$

where $t^{\pm}_{123}$ satisfy $t^{\pm}_{123} = V_{123} + V_{123}G_0^{\pm}t^{\pm}_{123}$ so $G^{\pm}_{123}V_{123} = G_0^{\pm}t^{\pm}_{123}$, $V_{123}|\phi^{\pm}_{123}\rangle = t^{\pm}_{123}|\phi\rangle$, and $|\phi^{\pm}_{123}\rangle = (1 + G_0^{\pm}t^{\pm}_{123})|\phi\rangle$.

It is clear from (4.13) and also from simple rearrangement of the differential equations that there is a set of plane wave spurious solutions which span $\mathscr{S}$. Under the appropriate L^2 assumption, the spectral and semigroup properties described previously again hold for this operator, which is equivalent to

$$\begin{pmatrix} H & 0 & 0 & 0 \\ 0 & H_0 & 0 & 0 \\ 0 & 0 & H_0 & 0 \\ 0 & 0 & 0 & H_0 \end{pmatrix}.$$

V. DISCUSSION

We briefly review the discussion of L'Huillier *et al.*[15] on the componentwise interpretation of the asymptotic two-cluster scattering solutions as this gives further insight into their nature. These sorts of considerations also lead to simple deductions on the nature of the spurious wavelike solutions compatible with our findings. These results are of more general applicability, as will be observed with regard to the N-particle Faddeev-like equations of the above authors. In fact, the Faddeev equations considered here are just one example of a wave-function formulation of many-particle scattering theory where the components of the asymptotic two-cluster scattering solutions are related to the Hilbert space solution by operators acting as asymptotic filters in various asymptotic regions, i.e., selecting specific types of outgoing waves (see Vanzani *et al.*[32]).

For the spatially-infinite Faddeev equation of Sec. III, the filter operators are just those used for the imbedding of the corresponding scattering solutions, i.e.,

$$F_j(E) = G_0^{\pm}(E)V_j \quad j=1,2,3, \tag{5.1}$$

so $|\Psi_j\rangle = F_j|\Psi\rangle$. Since V_j is zero outside the j-tube,[15] $|\Psi_j\rangle$ must satisfy $(E-T)|\Psi_j\rangle = 0$ there, and thus for the $\alpha = 1, 2, 3$ scattering solutions corresponds to a (hyper-) spherical breakup wave distribution among all three components. From the differential form of Faddeev's equation, for any eigenvector,

$$(E - T - V_j)|\Psi_j\rangle = S_j^F, \tag{5.2}$$

where the Faddeev source $S_j^F = V_j\Sigma_{k\neq j}|\Psi_k\rangle$ is confined to the j tube. Thus outside the j tube, $|\Psi_j\rangle$ satisfies $(E-T)|\Psi_j\rangle = 0$, which can correspond to the breakup part of a scattering solution or a spurious plane wave solution. The nonspurious part of $|\Psi_j\rangle$ evolves under H_j asymptotically in the j tube and thus supports bound states only in channel j.

If we consider the scattering solutions of the four-channel Faddeev equations, then the choice of asymptotic condition for the incoming part can always be made to give the incoming wave function components the appropriate physical interpretation (including the breakup, i.e., choose $j^* = 0$). Also, only $|\Psi_j\rangle$ can support j channel bound states in the outgoing part of the solution. For $\Psi_{0(0)}$ or $\Psi^{\pm}_{\alpha}$ $\alpha = 1, 2, 3$ where $E > 0$, there will, however, be a (hyper-) spherical outgoing breakup wave distributed between all four components, thus destroying the "perfect" componentwise interpretation.[33]

The N-particle Faddeev-like equations of L'Huillier *et al.* have the form

$$(E - (T + \mathscr{V}_\gamma))(\Psi)_\gamma = \mathscr{V}_\gamma\sum_\alpha(1-\delta_{\gamma,\alpha})(\Psi)_\alpha, \tag{5.3}$$

where γ and α are two-cluster channels and $\mathscr{V}_\gamma$ is the irredu-

cible γ-connected potential. The asymptotic two-cluster scattering solutions (and true N-particle bound state solutions) may be imbedded into solutions of the above equation using the filter operator $F_\gamma(E) = G_0^{\pm}(E)\mathscr{V}_\gamma$. For scattering solutions, $(\Psi)_\gamma$ includes a γ-bound-state part (should it exist) in the γ tube as well as finer-clustered parts in appropriately larger regions. By inspection we see that these equations also have a set of plane wave component spurious solutions. Without a demonstration of the imbedding of various multicluster scattering solutions, a complete spectral theory for the operator corresponding to (5.3) is not available.

Reviewing the results presented, we note that the Faddeev type channel-space Hamiltonians examined here provide the first example of the postulated scalar spectral structure for general channel-space Hamiltonians[5] (except in certain "accidental" cases). For a spatially infinite system with pairwise interactions (Sec. III) the operator is particularly simple, having no normalizable spurious solutions and having a real spectrum. Furthermore, the wavelike spurious solutions have the simplest possible structure for the three-channel, three-particle case, being plane wavelike everywhere rather than just asymptotically. The second example of Sec. IV is more indicative of the general case, where normalized spurious solutions may also exist (although this case is still special in that the solutions have real rather than complex eigenvalues). The technique of elucidating the channel-space Hamiltonian structure by presenting an equivalent operator with simple structure has broader applicability except that normal operators must in general be used.[34]

For both infinite and spatially confined systems, examples of the possible breakdown of the scalar spectral property have been given. A normalizable physical eigenvector is "replaced" by a spurious one, as has been anticipated from spectral theoretic arguments for general channel-space Hamiltonians.[5] The method of construction of appropriate generalized eigenvectors is also quite general, given a basis property of the spurious solutions on $\mathscr{S}$.

In future work, the nice scalar spectral property of the Faddeev Hamiltonian will be a powerful tool in analyzing the structure and spectral theory of related Hamiltonians, e.g., the three-particle BKLT choices.[34] Spurious multipliers are used here as intertwining operators.

APPENDIX A

We review some results developed previously[5] which relate the imbedding of H eigenvectors to the completeness and basis properties of H eigenvectors. If the physical and spurious eigenvectors are complete on the channel space, then it is necessary for all of the Hilbert space eigenvectors of H to be imbedded into those of H (strictly, "almost all" for continuous eigenvalues). There are also partial converses to this result. Suppose that all the eigenvectors of H are complete, so any vector in H can be approximated in norm by a certain class of linear combinations of these eigenvectors. Suppose, first, that the corresponding approximating linear combinations of channel-space eigenvectors are convergent (a trivial result if all the eigenvalues are discrete, i.e., the spatially-confined case[5]). Then we have the physical channel-space eigenvectors together with any complete set on $\mathscr{S} = \{\Psi \in \mathscr{C} : \Sigma_\alpha | \Psi_\alpha \rangle = 0\}$ are complete on $\mathscr{C}$. Second, suppose that for any convergent linear combination of eigenvectors of H, the corresponding linear combination of channel-space eigenvectors is convergent in norm. Then we have that the physical channel-space eigenvectors together with any basis for $\mathscr{S}$ form a basis for $\mathscr{C}$. These results are used in Secs. II, III, and IV.

APPENDIX B

An operator T for which there exists a countably additive resolution of the identity $\{\mathsf{E}(\delta)\}$ is called spectral. In particular, such bounded projections commute with each other, with T and $\mathsf{E}(\phi) = 0$, $\mathsf{E}(\mathbb{C}) = 1$. Such operators may be decomposed as follows:

$$\mathsf{T} = \mathsf{S} + \mathsf{N},$$

where $\mathsf{S} = \int \lambda\, \mathsf{E}(d\lambda)$ is the scalar part and N is quasinilpotent, i.e.,

$$\lim_{n\to\infty} \| |\mathsf{N}^n| \|^{1/n} = 0.$$

$\{\mathsf{E}(\delta)\}$ commute with both S and N.

If $f(\ )$ is analytic on an open set $\Delta(\mathsf{T})$ containing the spectrum $\sigma(\mathsf{T})$ of T, then we have the functional calculus (formally)

$$f(\mathsf{T}) = \sum_{n=0}^{\infty} \left(\frac{\mathsf{N}^n}{n!}\right) \int_{\Delta(\mathsf{T})} f^{(n)}(\lambda)\, \mathsf{E}(d\lambda)$$

and

$$f(\mathsf{S}) = \int f(\lambda)\, \mathsf{E}(d\lambda).$$

We say a spectral operator T is to type m if $\mathsf{N}^{m+1} = 0$. If $m < \infty$, then the residual spectrum $R\sigma(\mathsf{T}) = \emptyset$. Type '0' spectral operators are called scalar spectral, e.g.,

$n \times n$ matrices are spectral

normal operators are scalar spectral,

S is scalar spectral.

Sufficient conditions for the spectral property have been described by Dunford and Schwartz.[21] Direct verification of these is, however, expected to be extremely difficult for channel-space Hamiltonians (Chandler[35]). An alternative characterization is more convenient. If T is spectral and the spectrum is denumerable, then every vector in the space has an unconditionally convergent expansion in terms of "generalized eigenvectors" Ψ_n say. If T is type m, then these satisfy

$$(\lambda_n \mathsf{I} - \mathsf{T})^{m+1} \Psi_n = 0.$$

These ideas extend in the usual "weak" fashion to the case where a continuous spectrum is present. Thus for scalar spectral operators, e.g., H_F, the standard type of eigenvector expansion is valid. We shall show that the more general type 1 operators are relevant to the analysis of channel-space Hamiltonians where, for example, not all the Hilbert space Schrödinger equation solutions are imbedded into physical eigenvectors.

APPENDIX C

Here we investigate a situation where the scalar spectral property of the spatially confined Faddeev Hamiltonian H_F could breakdown. This is the case where one or more eigenvalues of H and H_e accidentally coincide, possibly causing the simple imbedding procedure for the corresponding H eigensolutions not to be valid. Specifically, suppose that

$$E_n = E^0_m = E(\kappa), \text{ say, where } n\in\mathcal{N}_\kappa,\ m\in\mathcal{M}_\kappa,$$

where $\mathcal{N}_\kappa$ and $\mathcal{M}_\kappa$ are finite sets (for each κ).

To understand the cause of the breakdown of imbedding, it is instructive to consider the above case as the limit of a sequence of well-behaved problems (as discussed in Sec. II). We perturb H_e and H by $\epsilon\tilde{V}_e$ to give $\tilde{H}_e$ and $\tilde{H}$ with noncoincident eigenvalues $\tilde{E}^0_m$ and $\tilde{E}_n$ and corresponding eigenvectors $|\tilde{\phi}(m)\rangle$ and $|\tilde{\Psi}(n)\rangle$, respectively. Thus $\tilde{E}_n - \tilde{E}^0_m \to 0$ as $\epsilon\to 0$ if $n\in\mathcal{N}_\kappa$, $m\in\mathcal{M}_\kappa$. We are particularly interested in the behavior of $\tilde{\Psi}(n)$ with $n\in\mathcal{N}_\kappa$ as $\epsilon\to 0$. Now, for $n\in\mathcal{N}_\kappa$,

$$\begin{aligned}|\tilde{\Psi}(n)\rangle &= \tilde{G}_e(\tilde{E}_n)V|\tilde{\Psi}(n)\rangle \\ &= \sum_{m\in\mathcal{M}_\kappa}\frac{\langle\tilde{\phi}(m)|\,V|\tilde{\Psi}(n)\rangle}{\tilde{E}_n-\tilde{E}^0_m}|\tilde{\phi}(m)\rangle \\ &\quad + \tilde{\mathcal{G}}_e(\tilde{E}_n)V|\tilde{\Psi}(n)\rangle,\end{aligned}$$

where

$$\tilde{G}_e(z) = (z-\tilde{H}_e)^{-1} = \sum_{m\in\mathcal{M}_\kappa}\frac{|\tilde{\phi}(m)\rangle\langle\tilde{\phi}(m)|}{z-\tilde{E}^0_m} + \tilde{\mathcal{G}}_e(z),$$

so $\langle\tilde{\phi}(m)|\,V|\tilde{\Psi}(n)\rangle/(\tilde{E}_n-\tilde{E}^0_m)\to\langle\phi(m)|\Psi(n)\rangle$, a finite constant, as $\epsilon\to 0$.

From Sec. II, the components of the imbedded channel-space solution $\tilde{\Psi}(n)$, $n\in\mathcal{N}_\kappa$, are given by

$$|\tilde{\Psi}_j(n)\rangle = \sum_{m\in\mathcal{M}_\kappa}\frac{\langle\tilde{\phi}(m)|V_j|\tilde{\Psi}(n)\rangle}{\tilde{E}_n-\tilde{E}^0_m}|\tilde{\phi}(m)\rangle + \tilde{\mathcal{G}}_e(\tilde{E}_n)V_j|\tilde{\Psi}(n)\rangle$$

and

$$|\tilde{\phi}(m)\rangle\to|\phi(m)\rangle,$$

$$\tilde{\mathcal{G}}_e(\tilde{E}_n)V_j|\tilde{\Psi}(n)\rangle\to\mathcal{G}_e(E_n)V_j|\Psi(n)\rangle,$$

$$\frac{\langle\tilde{\phi}(m)|\,V_j|\tilde{\Psi}(n)\rangle}{\tilde{E}_n-\tilde{E}^0_m}\to\infty,\quad j=1,2,3,$$

as $\epsilon\to 0$. Consequently if $n\in\mathcal{N}_\kappa$,

$$\operatorname{dist}\left(\frac{\tilde{\Psi}(n)}{\|\tilde{\Psi}(n)\|},\text{span }\{\phi^i(m)\ i=1,2,\ m\in\mathcal{M}_\kappa\}\right)\to 0 \text{ as } \epsilon\to 0,$$

i.e., the normalized form of the physical solution $\tilde{\Psi}(n)$ coalesces with the spurious solutions $\tilde{\phi}^i(m)$ $i=1,2$, $m\in\mathcal{M}_\kappa$ as $\epsilon\to 0$.

Let us now return to the analysis of the limiting situation described above. Suppose that there are no imbedded physical eigenvectors corresponding to $|\Psi(n)\rangle$ for $n\in\hat{\mathcal{N}}_\kappa(\subseteq\mathcal{N}_\kappa)$ for each κ. First observe that for such n, if we choose any $\Psi(n)$ such that $\Sigma_{j=1}^3|\Psi_j(n)\rangle = |\Psi(n)\rangle$, then

$$(\mathsf{H}_F - E(\kappa))\Psi(n)\in\mathcal{S}.$$

Further, it is easily verified that we can modify $\Psi(n)$ by adding a suitable linear combination of the $\phi^i(m)$ $i=1,2$, $m\notin\mathcal{M}_\kappa$, so that, specifically,

$$(\mathsf{H}_F - E(\kappa))\Psi(n) = \sum_{i=1}^{2}\sum_{m\in\mathcal{M}_\kappa}C^n_{i,m}\,\phi^i(m)$$

for some $C^n_{i,m}$ not all zero. With such a choice we have

$$(\mathsf{H}_F - E(\kappa))^2\Psi(n) = 0.$$

Since H_F couples $\Psi(n)$ and $\phi^i(m)$ for $n\in\hat{\mathcal{N}}_\kappa$, $m\in\mathcal{M}_\kappa$, it is not scalar spectral. However, given the l^2 assumption, it could at worst be spectral of finite type since the coupling is on a finite-dimensional subspace and the above construction of the generalized eigenvectors $\Psi(n)$ shows that it is type 1. This results from the summation property of H_F and the completeness of the spurious solutions. To elucidate this structure we observe that since $\{\Psi(n),\phi^i(m)\}$ provides a basis for $\mathscr{C}$, we may uniquely define a set of biorthogonal dual vectors $\{\zeta^i(n),\zeta^{i'}(m)\}$. Clearly

$$(\zeta^i(n))_j = \langle\Psi(n)|,\quad j=1,2,3$$

and $(\mathsf{H}'_F - E_n)\zeta^i(n) = 0'$.

It is readily verified that, provided $m\notin\mathcal{M}_\kappa$ for any κ,

$$(\zeta^{i'}(m),(\mathsf{H}_F - E^0_m)\Psi) = 0 \text{ for } \Psi = \phi^j(m),\ \Psi(n),$$

where $n\notin\hat{\mathcal{N}}_\kappa$ for any κ, and if $n\in\hat{\mathcal{N}}_\kappa$ then

$$\begin{aligned}&(\zeta^{i'}(m),(\mathsf{H}_F - E^0_m)\Psi(n)) \\ &= \left(\zeta^{i'}(m),\sum_{i=1}^{2}\sum_{p\in\mathcal{M}_\kappa}C^n_{i,p}\phi^i(p) + \sum_{i=1}^{2}\sum_{p\in\mathcal{M}_\kappa}(E^0_p - E^0_m)\Psi(n)\right) \\ &= 0.\end{aligned}$$

Consequently, $(\mathsf{H}'_F - E^0_m)\,\zeta^{i'}(m) = 0'$ (provided $m\notin\mathcal{M}_\kappa$).

However if $m\in\mathcal{M}_\kappa$ for some κ, then

$$(\zeta^{i'}(m),(\mathsf{H}_F - E^0_m)\Psi(n)) = C^n_{i,m} \text{ if } n\in\mathcal{N}_\kappa$$

so $\zeta^{i'}(m)$ may not be an eigenvector of H'_F. However, it is easily demonstrated that

$$(\mathsf{H}'_F - E^0_m)^2\zeta^{i'}(m) = 0'.$$

By way of example, consider the simplest case, where the only eigenvalue coincidence is $E_{n^*} = E^0_{m^*} = E_*$, say. Suppose that the imbedding for $|\Psi(n^*)\rangle$ breaks down; then we construct $\Psi(n^*)$ so that

$$(\mathsf{H}_F - E_*)\Psi(n^*) = C_1\phi^1(m^*) + C_2\phi^2(m^*).$$

It is appropriate here to replace $\phi^i(m^*)$ with linearly independent linear combinations $\hat{\phi}^i(m^*)$ so that $\hat{\phi}^1(m^*) = C_1\phi^1(m^*) + C_2\phi^2(m^*)$. Then if $\zeta^i(n^*)$, $\hat{\zeta}^{1'}(m^*)$, $\hat{\zeta}^{2'}(m^*)$ are the biorthogonal duals, $\hat{\zeta}^{2'}(m^*)$ is now an eigenvector of H'_F, and H_F has the structure

$$\begin{array}{c} \\ \zeta^i(n^*) \\ \hat{\zeta}^{1'}(m^*) \\ \hat{\zeta}^{2'}(m^*)\end{array}\begin{array}{c}\begin{array}{ccc}\Psi(n^*) & \hat{\phi}^1(m^*) & \hat{\phi}^2(m^*)\end{array} \\ \begin{pmatrix} E_* & 0 & 0 \\ 1 & E_* & 0 \\ 0 & 0 & E_*\end{pmatrix}\end{array}.$$

In the notation of Appendix B, $\mathsf{E}(E_n)$, $n\neq n^*$ and $\mathsf{E}(E^0_m)$, $m\neq m^*$ are simply the projection operators onto the corresponding H_F-invariant eigenspaces. The resolution of the identity is completed by

$$\mathsf{E}(E_*) = (\Psi(n^*)\zeta^i(n^*) + \hat{\phi}^1(m^*)\hat{\zeta}^{1'}(m^*)) + \hat{\phi}^2(m^*)\hat{\zeta}^{2'}(m^*),$$

which also decomposes as a sum of two H_F-invariant projec-

tion operators. Finally,

$$\mathsf{N} = (\mathsf{H}_F - E_*)\mathsf{E}(E_*) = \hat{\phi}^1(m^*)\xi'(n^*),$$

and, of course, $\mathsf{N}^2 = 0$.

Various other specific cases can be analyzed similarly.

APPENDIX D

Suppose that the L^2 assumption for H_F of Sec. III holds. Then H_F is real eigenvalue scalar spectral and satisfies a *mean ergodic theorem*. Explicitly, the following holds. Let $\mathsf{E}(E_n)$ denote the projection operator onto the bound-state eigenvectors with eigenvalue E_n. Then

$$\mathsf{E}(E_n) = \underset{(t_2-t_1)\to\infty}{\text{s-lim}} \frac{1}{t_2 - t_1}\int_{t_1}^{t_2} e^{\pm itH_F} e^{\mp itE_n}\, dt.$$

To prove this result directly one first expresses a vector Ψ in $\mathscr{C}$ explicitly as a linear combination of the basis eigenvectors of H_F. Then the Lebesgue dominated convergence theorem may be used to show that

$$\left|\left|\mathsf{E}(E_n)\Psi - \frac{1}{t_2 - t_1}\int_{t_1}^{t_2} e^{\pm itH_F} e^{\mp itE_n}\Psi\, dt\right|\right| \to 0$$

as $t_2 - t_1 \to \infty$.

Alternatively, the result may be proved using (3.28) and the mean ergodic theorem for the self-adjoint operator

$$\begin{pmatrix} H & 0 & 0 \\ 0 & H_0 & 0 \\ 0 & 0 & H_0 \end{pmatrix}.$$

It is easily checked that for any $\Psi \in \mathscr{C}$ such that $\Sigma_\alpha |\Psi_\alpha\rangle = |\Psi(n)\rangle$ we have $\mathsf{E}(E_n)\Psi = \Psi(n)$.

Consequently the mean ergodic theorem provides an alternate imbedding procedure for the bound-state solutions. We remark that the existence of such an imbedding for general channel-space Hamiltonians is at present unresolved.

APPENDIX E

In the expression (3.29) for the spurious dual eigenvectors we must examine singular expressions of the form $(\hat{\xi}^{i'}(k), \Psi_\alpha^\pm(\mathbf{k}^\alpha, m))$. It is convenient to introduce a Jacobi decomposition of the wave vectors, i.e., $\mathbf{k} = (\mathbf{k}_1, \mathbf{k}_{23}) = \cdots$, where $\mathbf{k}_1$ is the momentum of 1 relative to the pair 23 and $\mathbf{k}_{23}$ the momentum of 2 relative to 3. For the corresponding kinetic energy $E = E_1 + E_{23} = \cdots$, and plane wave $|\phi(\mathbf{k})\rangle = |\phi(\mathbf{k}_1)\rangle \otimes |\phi(\mathbf{k}_{23})\rangle = \cdots$.

It is easily verified from (3.8) and (3.10) that

$$(\Psi_\alpha^\pm(\mathbf{k}^\alpha, m))_j = \delta_{\alpha j}|\phi(\mathbf{k}^\alpha)\rangle \otimes |\phi_m\rangle + G_0^\pm t_j^\pm G_0^\pm V^j |\Psi_\alpha^\pm(\mathbf{k}^\alpha, m)\rangle, \qquad \alpha = 1, 2, 3,$$

so, for example,

$$(\hat{\xi}^{i'}(\mathbf{k}), \Psi_1^\pm(\mathbf{k}^1, m)) = \chi^i{}_1 \delta(\mathbf{k}_1 - \mathbf{k}^1)\langle\phi(\mathbf{k}_{23})|\phi_m(23)\rangle + \sum_{j\neq j^*} \chi_j^i \langle\phi(\mathbf{k})|G_0^\pm t_j^\pm G_0^\pm V^j|\Psi_1^\pm(\mathbf{k}^1, m)\rangle.$$

From (3.14) and noting that $\chi^i_{j^*} = 0$ eliminates the $\delta(\mathbf{k} - \mathbf{k}^0)$ term, we have

$$\begin{aligned}(\hat{\xi}^{i'}(\mathbf{k}), \Psi_{0\hat{0}^*}^\pm(\mathbf{k}^0)) &= \chi^i{}_1 [\delta(\mathbf{k}_1 - \mathbf{k}_1^0)\langle\phi(\mathbf{k}_{23})|\hat{G}_0^\pm(E^0_{23})\hat{t}_1(E^0_{23})|\phi(\mathbf{k}^0_{23})\rangle \\ &\quad + \langle\phi(\mathbf{k})|G_0^\pm t_1^\pm G_0^\pm V^1|\Psi_{0\hat{0}^*}^\pm(\mathbf{k}^0)\rangle] \\ &\quad + (1\to2\to3\to1) + (1\to3\to2\to1),\end{aligned}$$

and here $\hat{G}_0^\pm$ and $\hat{t}_j$ are the true two-body operators corresponding to $G_0^\pm$ and $t_j^\pm$. The operators $G_0^\pm$ and $\hat{G}_0^\pm$ appearing to the left above may be decomposed into Cauchy principal-value and energy delta-function parts.[31] This makes explicit all delta functions in the above expressions, since the remaining operators are connected. The detailed behavior of the regular terms appearing depends on the nature of the potentials.[27]

APPENDIX F

Some results for the dual eigenvectors in the spatially infinite case of Sec. III are presented here, omitting eigenvector labels where possible, for simplicity. By definition, for $\alpha = 1, 2, 3$,

$$[\xi_\alpha^{\pm\prime}]_j = \langle\Psi_\alpha^\pm|, \quad \forall j$$

so $[\xi_\alpha^{\pm\prime}]_j \sim \langle\phi(\alpha)| \otimes \langle\phi_m|$, $\forall j$ asymptotically where $|\phi(\alpha)\rangle$ is a plane wave for particle α, and $|\phi_m\rangle$ is a bound state in the other particles. However,

$$\xi_\alpha^{\pm\prime} = \xi'_\alpha + \xi_\alpha^{\pm\prime} V_F G_0^\mp,$$

where $[\xi'_\alpha]_j = \delta_{\alpha j}\langle\phi(\alpha)| \otimes \langle\phi_m|$. Also, since

$$[\xi_0^{\pm\prime}]_j = \langle\Psi_0^\pm|, \quad \forall j,$$

we have that $[\xi_0^{\pm\prime}]_j \sim \langle\phi|, \forall j$ or $\xi_0^{\pm\prime} \sim \chi^{3\prime}\langle\phi|$ in the breakup region (here $|\phi\rangle$ is a plane wave) and

$$\xi_0^{\pm\prime} = \xi_0^{\pm\prime} + \xi_0^{\pm\prime} V_F G_0^\mp,$$

where $[\xi_0^{\pm\prime}]_j = \langle\phi_j{}^\pm|$, $\forall j$ so $\xi_0^{\pm\prime}\cdot(E - \mathsf{H}_0) = 0'$ and $\xi_0^{\pm\prime} \sim \chi^{3\prime}\langle\phi|$ in the breakup region. The above mentioned integral equations for $\xi_\alpha^{\pm\prime}$ and $\xi_0^{\pm\prime}$ reduce to the LS–GT equations if we explicitly set all the components of these vectors equal.

For the spurious duals, from biorthogonality, we must have

$$\xi^{\pm i'} \sim \chi^{i'}\langle\phi|, \quad i = 1, 2,$$

in the breakup region. They must satisfy the integral equations

$$\xi^{\pm i'} = \xi^{\pm i'} + \xi^{\pm i'} V_F G_0^\mp,$$

where $[\xi^{\pm i'}]_j = \chi_j^i \langle\phi_j{}^\pm|$, $\forall j$.

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Quantum-mechanical scattering by impenetrable periodic surfaces

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(Received 20 January 1981; accepted for publication 1 May 1981)

In this paper, we investigate the existence and completeness of the wave operators $W_{\pm} = \text{s-lim}_{t \to \pm\infty} \exp(itH)\mathscr{P}\exp(-itH_0)$ corresponding to the quantum-mechanical scattering of nonrelativistic particles by certain classes of impenetrable noncompact surfaces bounding domains $\Omega \subset \mathbb{R}^\nu (\nu \geqslant 2)$ which contain a half-space and are contained in another half-space. Here, H_0 is the usual negative (distributional) Laplacian $-\Delta$ in $\mathscr{H}_0 = L^2(\mathbb{R}^\nu)$, H is the negative Dirichlet Laplacian in $\mathscr{H} = L^2(\Omega)$, and $\mathscr{P}$ is an appropriate identification operator. Under these conditions, we prove by elementary methods that $W_{\pm}$ exist as partially isometric operators whose initial sets have a transparent physical meaning. Suppose now that the domain $\Omega \subset \mathbb{R}^\nu$ also has the periodicity property $(\tilde{x},x_\nu)\in\Omega \Rightarrow (\tilde{x}+l,x_\nu)\in\Omega$ when l ranges over a Bravais lattice in $\mathbb{R}^{\nu-1}$, where we write $x\in\mathbb{R}^\nu$ as $(\tilde{x},x_\nu)$, with $\tilde{x}\in\mathbb{R}^{\nu-1}$ and $x_\nu\in\mathbb{R}$. Then (a) $\text{Ran}\,W_{\pm} = \mathscr{H}_{\text{scatt}}(H)$ and (b) $W_{\pm}$ are asymptotically complete, in the sense that $\mathscr{H} = \mathscr{H}_{\text{scatt}}(H) \oplus \mathscr{H}_{\text{surf}}(H)$. Here, $\mathscr{H}_{\text{scatt}}(H)$ and $\mathscr{H}_{\text{surf}}(H)$ are suitably defined subspaces of scattering and surface states of $\mathscr{H}$, respectively. Results (a) and (b) are proved by reducing the original scattering problem to a family of "scattering" problems in a periodicity cell of Ω, using direct-integral methods, and by then using methods analogous to those of Lyford. The present work constitutes a rigorous foundation for the theory of scattering of low-energy atomic beams by crystal surfaces, considered as impenetrable periodic barriers. Our methods should also be applicable to rigorous investigations of classical scattering by periodic surfaces with Dirichlet or Neumann boundary conditions.

PACS numbers: 03.65.Nk

I. INTRODUCTION

In this paper, we give a time-dependent treatment of the quantum-mechanical scattering of nonrelativistic particles by certain impenetrable surfaces, and particularly by periodic surfaces. In this context, impenetrable means that the relevant wavefunctions obey the (generalized) homogeneous Dirichlet condition at the surfaces considered. Quantum-mechanical scattering of nonrelativistic particles by impenetrable surfaces has been successfully used,[1] at the level of formal stationary scattering theory, as a model for low-energy atomic-beam scattering by crystal surfaces. The present work initiates the study of such scattering phenomena by rigorous methods. We have also applied the methods of this paper to investigate rigorously classical wave scattering by periodic surfaces with the homogeneous Dirichlet or Neumann boundary conditions. The results will be reported in a subsequent publication.

Our point of view will be that of time-dependent scattering theory with two Hilbert spaces. The "unperturbed" Hamiltonian H_0 is the negative distributional Laplacian in $\mathscr{H}_0 = L^2(\mathbb{R}^\nu)$ $(\nu \geqslant 2)$ and the "perturbed" Hamiltonian H is the negative Dirichlet Laplacian $-\Delta_D(\Omega)$ in $\mathscr{H} = L^2(\Omega)$, where $\Omega \subset \mathbb{R}^\nu$ is an appropriate exterior domain and $-\Delta_D(\Omega)$ acts as $-\Delta$ on suitable elements of $\mathscr{H}$ vanishing on $\partial\Omega$ in a generalized sense. The class of exterior domains considered here is such that Ω always contains a space and is contained in a half-space. Most of our discussions refer to the case when, in addition, Ω has the periodicity property that $(\tilde{x},x_\nu)\in\Omega \Rightarrow (\tilde{x}+l,x_\nu)\in\Omega$, where l ranges over a general in $\mathbb{R}^{\nu-1}$ and where we have written $x\in\mathbb{R}^\nu$ as $(\tilde{x},x_\nu)$, with $\tilde{x}\in\mathbb{R}^{\nu-1}$ and $x_\nu\in\mathbb{R}$. *No smoothness or regularity conditions are imposed on $\partial\Omega$ in this paper.*

It is surprising that the time-dependent scattering problem posed by such exterior domains has apparently not been treated in the literature (even at the formal level), except for essentially trivial cases, as a perturbation of H_0 by the relevant noncompact surface, although this is very natural from a physical viewpoint.

We proceed to describe the organization of the present paper.

In Sec. II, we state and prove Theorem 2.1, which applies when the domain $\Omega \subset \mathbb{R}^\nu$ of interest contains a half-space and is itself contained in one, but Ω need not have any periodicity properties. This theorem asserts that the wave operators

$$W_{\pm} = W_{\pm}(H,H_0) = \text{s-lim}_{t\to\pm\infty} \exp(itH)\mathscr{P}\exp(-itH_0)$$

appropriate to scattering in such exterior domains are partially isometric, where $\mathscr{P}$ is a suitable identification operator. The initial sets of $W_{\pm}$ have transparent physical meanings.

The main results of the paper, Theorems 3.1 and 3.2, are stated in Sec. III, where the strategy of their proofs is also discussed. These theorems apply when Ω, besides being as stated in the last paragraph, also possesses the periodicity property mentioned above. Theorem 3.1 asserts that $\text{Ran}\,W_{\pm}$ are equal to the subspace $\mathscr{H}_{\text{scatt}}(H)$ of scattering states, consisting of those $f\in\mathscr{H}$ which are evanescent from each region bounded by $\partial\Omega$ and a hyperplane $x_\nu = \text{const}$. (The coordinate x_ν is as above.) One expects that $\mathscr{H}_{\text{scatt}}(H)$ is

generally a proper subspace of the subspace of absolute continuity of $\mathscr{H}$ with respect to H. Theorem 3.2 asserts that $W_\pm$ are asymptotically complete in the sense that $\mathscr{H}_{\text{scatt}}(H)$ is the orthogonal complement, with respect to $\mathscr{H}$, of the subspace $\mathscr{H}_{\text{surf}}(H)$ of surface states. $\mathscr{H}_{\text{surf}}(H)$ consists of those $f \in \mathscr{H}$ which for all time remain "close" to $\partial\Omega$ in a suitable sense. Our definition of $\mathscr{H}_{\text{scatt}}(H)$, as well as our completeness results, are analogous to the corresponding definition and results in a paper of Davies and Simon,[2] dealing with scattering by crystals. (The physical problem considered in the present paper is different from those considered in Ref. 2 and our methods of proof, except for the use of direct-integral procedures, are mostly very different from theirs.)

The remaining sections, Secs. IV–VIII, are devoted to proving Theorems 3.1 and 3.2 by means of a series of lemmas. The proof of Theorem 3.1 involves two steps. The first is to replace the original scattering problem (H_0,H) by another time-dependent scattering problem (H^0,H), where H^0 is the negative Dirichlet Laplacian $-\Delta_D(\Omega^0)$, Ω^0 denoting an appropriate half-space containing Ω. The advantage of the latter problem over the original one, from the standpoint of the methods used here, is that H is a less "drastic" perturbation of H^0 than of H_0. The second step is to exploit the periodicity of Ω to reduce the study of the problem (H^0,H) to that of a family of "scattering" problems in an external domain ω which is a periodicity cell of Ω, and is, therefore, generally a distorted cylinder. We handle this family of problems by mathematical techniques analogous to those used by Lyford in his studies of the spectral and scattering theory of distorted cylinders[3–5] and distorted periodic waveguides.[6]

The second step mentioned above relies on direct-integral methods, whose usefulness in other scattering problems involving periodicity properties is well recognized.[7] The assumed periodicity of Ω allows one to represent $\mathscr{H}$ as a constant-fiber direct integral $\int_{\mathscr{G}}^{\oplus} L^2(\omega)\,d\mu$, where $d\mu$ is proportional to Lebesgue measure in $\mathbb{R}^{\nu-1}$ and $\mathscr{G} \subset \mathbb{R}^{\nu-1}$ is a certain open parallellipiped. As explained in Sec. V, in order to prove Theorem 3.1 it suffices (modulo standard measure-theoretic technicalities) to establish that the wave operators

$$\text{s-lim}_{t \to \pm\infty} \exp(ith_\theta)\eta \exp(-ith_\theta^0) \quad (\theta \in \mathscr{G})$$

which are complete in the usual sense,[9] where $\{h_\theta^0, \theta \in \mathscr{G}\}$ and $\{h_\theta, \theta \in \mathscr{G}\}$ are families of self-adjoint operators in terms of which H and H^0 can be represented as $\int_{\mathscr{G}}^{\oplus} h_\theta\,d\mu$ and $\int_{\mathscr{G}}^{\oplus} h_\theta^0\,d\mu$, respectively, and η is an identification mapping. The completeness of these wave operators is proved in Sec. V by using a version of well-known theorems of Birman and Belopol'skii[10] due to Lyford,[11] together with properties of the h_θ^0's and h_θ's discusssed in Sec. IV.

In Sec. VI, we prove a lemma which states, in particular, that the point spectrum of each h_θ is nowhere dense in $\mathbb{R}$. In Sec. VII, we establish a lemma giving a bound of the $L^2(\omega)$-norm of $(h_\theta - \zeta)^{-1}f$ for every θ and a certain dense set of f's as ζ approaches suitable points of $\mathbb{R}$. These two lemmas are applied in Sec. VII to show that each h_θ has an empty singular continuous spectrum. The latter result plays an essential role in the proof of Theorem 3.2 which is given in Sec. VIII.

The function-space notation used in the paper is explained in Appendix A. Appendices B and C are devoted to stating and proving various results needed in the main text.

After completing this work, we learned of the recent study of Wilcox[13] on classical wave scattering by plane diffraction gratings with the homogeneous Dirichlet or Neumann boundary conditions. In that study, and in contrast to our approach, Wilcox constructs the relevant operators and proves their completeness by using his theory of Rayleigh–Bloch expansions.[14] He also derives a number of other results. In Ref. 13, the above completeness property is established under the hypothesis that no Rayleigh–Bloch surface waves exist. (These waves are analogous to the surface states considered in the present paper.)

II. EXISTENCE AND PARTIAL ISOMETRY OF WAVE OPERATORS FOR SCATTERING BY A GENERAL CLASS OF IMPENETRABLE NONCOMPACT SURFACES

Let Ω be a domain in $\mathbb{R}^\nu$ $(\nu \geqslant 2)$ such that

(I) $\mathbb{R}^{\nu-1} \times [\beta,\infty) \subset \Omega \subset \mathbb{R}^{\nu-1} \times [\alpha,\infty)$

for some $0 < \alpha < \beta < \frac{1}{2}$.

We will write the points of $\mathbb{R}^\nu$ as $(\tilde{x},x_\nu)$, with $\tilde{x} \in \mathbb{R}^{\nu-1}$ and $x_\nu \in \mathbb{R}$. Clearly, (I) implies that $\partial\Omega$ is contained in the "slice" $\alpha \leqslant x_\nu \leqslant \beta$. No conditions other than (I) will be imposed on the domain Ω in the present section.

Let

$$\mathscr{H}_0 = L^2(\mathbb{R}^\nu), \quad \mathscr{H} = L^2(\Omega),$$

and define the self-adjoint operators

$$H_0 = -\Delta, \quad H = \Delta_D(\Omega), \tag{2.1}$$

where Δ is the usual distributional Laplacian in $\mathscr{H}_0$ and $\Delta_D(\Omega)$ is the Dirichlet Laplacian in $\mathscr{H}$, acting by $-\Delta$ [15] on the (equivalence class of) functions in its domain, which is given by

$$D(\Delta_D(\Omega)) = L^2(\Delta;\Omega) \cap H_0^1(\Omega). \tag{2.2}$$

Here, $L^2(\Delta;\Omega)$ is the Hilbert space defined in the first paragraph of Appendix A and $H_0^1(\Omega)$ is the usual Sobolev space.

Definition: Let K_0 and K be self-adjoint operators in the respective Hilbert spaces $\mathscr{K}_0$ and $\mathscr{K}$, with K_0 having a purely absolutely continuous spectrum, and let $B: \mathscr{K}_0 \to \mathscr{K}$ be a bounded operator. Then the wave operators $W_\pm(K,K_0;B)$ are defined by

$$W_\pm(K,K_0;B) = \text{s-lim}_{t \to \pm\infty} \exp(itK)\,B \exp(-itK_0)$$

when they exist. [For all the wave operators $W_\pm(K,K_0;B)$ considered here, K_0 is an operator obeying the above spectral requirement.]

In this section, we discuss the wave operators

$$W_\pm = W_\pm(H,H_0) = W_\pm(H,H_0;\mathscr{P}), \tag{2.3}$$

as well as the operators $W_\pm(H,H_0;J)$, which is another way of writing $W_\pm$ which has certain well-known technical advantages. Here, $\mathscr{P}: \mathscr{H}_0 \to \mathscr{H}$ is given by

$$(\mathscr{P}f)(x) = f(x), \quad f \in \mathscr{H}_0, \ x \in \Omega, \tag{2.4}$$

and $J: \mathscr{H}_0 \to \mathscr{H}$ by

$$(Jf)(x) = j(x_\nu)\,f(x), \quad f \in \mathscr{H}_0, \ x = (\tilde{x},x_\nu) \in \Omega, \tag{2.5}$$

where $j \in C^\infty(\mathbb{R})$ satisfies the condition

$$j(y) = \begin{cases} 0, & y \leqslant \frac{1}{2}, \\ 1, & y \geqslant 1. \end{cases} \tag{2.6}$$

Theorem 2.1: (a) $W_\pm(H,H_0)$ exist and are equal to $W_\pm(H,H_0;J)$.

(b) $W_\pm(H,H_0)$ are partially isometric with initial sets

$$\mathscr{H}_\pm = \{f \in \mathscr{H}_0 : \hat{f}(k) = 0 \text{ for a.e. } k = (k_1,\ldots,k_\nu) \in \mathbb{R}^\nu \text{ with } k_\nu \lessgtr 0\}. \tag{2.7}$$

Remark: The assertion (b) of the theorem has a transparent physical interpretation. Intuitively, in order for a wavepacket f_t, evolving as $\exp(-itH_0)f$ for large negative times, to arrive "near" some point of $\partial\Omega$ at $t = 0$, its Fourier transform $\hat{f}_t$ must have for $t \to -\infty$ support intersecting the region of momentum space with $k_\nu < 0$ in a set of positive measure. Again intuitively, if a wavepacket g_t in Ω, which was "near" $\partial\Omega$ at $t = 0$, has been scattered, then the support of $\hat{g}_t$ must, for large positive times, intersect the momentum-space region with $k_\nu > 0$ in a set of positive measure.

Proof of Theorem 2.1: (a) Let $g \in \mathscr{S}(\mathbb{R}^\nu)$ be of the form

$$g(x) = g_1(\tilde{x})g_2(x_\nu). \tag{2.8}$$

Here, $g_1 \in \mathscr{S}(\mathbb{R}^{\nu-1})$ and the Fourier transform of g_2 is in $C_0^\infty(\mathbb{R}\setminus\{0\})$. Now, $g \in D(H_0)$ and $Jexp(-itH_0)g \in D(H)$ $(t \in \mathbb{R})$, where the second assertion follows by $\exp(-itH_0)g \in \mathscr{S}(\mathbb{R}^\nu)$ $(t \in \mathbb{R})$, (I), (2.1), (2.2), (2.5), (2.6), and $j \in C^\infty(\mathbb{R})$. Therefore,

$$\begin{aligned} &\left\| \frac{d}{dt}[\exp(itH)J\exp(-itH_0)g] \right\|_\Omega \\ &\quad = \|(HJ - JH_0)\exp(-itH_0)g\|_\Omega \\ &\quad \leqslant \|g_1\|_{\mathbb{R}} \cdot \{\|j''(x_\nu)\exp[it\Delta(\mathbb{R})]g_2\|_{\mathbb{R}} \\ &\qquad + 2\|j'(x_\nu)\exp[it\Delta(\mathbb{R})]g_2'\|_{\mathbb{R}}\}, \quad t \in \mathbb{R}, \end{aligned} \tag{2.9}$$

where the primes indicate differentiations with respect to x_ν, $\Delta(\mathbb{R})$ is the (distributional) Laplacian in $L^2(\mathbb{R})$, and $\|\cdot\|_A = \|\cdot\|_{L^2(A)}$ for each measurable set $A \subset \mathbb{R}^n$ $(n = 1,2,\ldots)$.

Since $j', j'' \in C_0^\infty(\mathbb{R})$ and since the Fourier transforms of g_2 and g_2' are in $C_0^\infty(\mathbb{R}\setminus\{0\})$, it follows[16] that each of the terms in the last line of (2.9) are $\leqslant$ const $|t|^{-(1+\epsilon)}$ for each $|t| > 1$ and $\epsilon > 0$, and hence that the norm in the first line of (2.9) is in $L^1((-\infty,-1)\cup(1,\infty))$ as a function of t. Whence, because the mapping $t \to (HJ - JH_0)\exp(-itH_0)g$ from $\mathbb{R}$ into $\mathscr{H}$ is continuous and the set of all g's of the form (2.8) is dense in $\mathscr{H}_0$, $W_\pm(H,H_0;J)$ exist.

By virtue of this result, it suffices to show that

$$\lim_{t \to \pm\infty} \|(J - \mathscr{P})\exp(-itH_0)g\|_\Omega = 0 \tag{2.10}$$

for each such g in order to conclude that $W_\pm(H,H_0)$ exist and are equal to $W_\pm(H,H_0;J)$. Now, by (2.4)–(2.6) and $j \in C^\infty(\mathbb{R})$, $((J - \mathscr{P})f)(x) = r(x)f(x)$ $(f \in \mathscr{H}_0,\ x \in \Omega)$, where $r \in C^\infty(\Omega)$ vanishes for $x_\nu \geqslant 1$. Hence, (2.10) follows by the same result[14] invoked above.

(b) We want to prove that

$$\|W_\pm f\|_\Omega^2 = \int_{\mathbb{R}^\nu, k_\nu \gtrless 0} |f(k)|^2 dk, \quad f \in \mathscr{H}_0. \tag{2.11}$$

To prove (2.11), we first remark that

$$\lim_{t \to \pm\infty} \|\exp(-itH_0)f\|_{\Omega^0\setminus\Omega}^2 = 0, \tag{2.12}$$

for each $f \in \mathscr{H}_0$, where

$$\Omega^0 = \mathbb{R}^{\nu-1} \times \mathbb{R}_+, \tag{2.13}$$

with $\mathbb{R}_+ = (0,\infty)$.

Equation (2.12) follows for $f \in \mathscr{H}_0$ of the form specified by (2.8) and the sentence following that equation by an argument of the same type as that used to estimate the large $|t|$ behavior of the expression in the last line of (2.9). A density argument completes the proof of (2.12).

As is well known,[17] the unitary operator Z_t: $\mathscr{H}_0 \to \mathscr{H}$ $(t \in \mathbb{R})$ with action

$$(Z_t f)(x) = (2it)^{-\nu/2}\exp(i|x|^2/4t)\hat{f}((2t)^{-1}x) \tag{2.14}$$

on each $f \in \mathscr{H}_0$, approximates $\exp(-itH_0)$ in the strong sense for $t \to \infty$:

$$\mathscr{H}_0\text{-}\lim_{t \to \pm\infty} [\exp(-itH_0) - Z_t] = 0. \tag{2.15}$$

Using, in particular, the unitarity of $\exp(-itH_0)$, (2.12), (2.14), and (2.15), we obtain

$$\begin{aligned} \|W_\pm f\|^2 &= \lim_{t \to \pm\infty} \|\exp(-itH_0)f\|_\Omega^2 \\ &= \lim_{t \to \pm\infty} \|\exp(-itH_0)f\|_{\Omega^0}^2 \\ &= \lim_{t \to \pm\infty} \|Z_t f\|_{\Omega^0}^2 = \int_{k_\nu \gtrless 0} |\hat{f}(k)|^2 dk. \ \blacksquare \end{aligned}$$

The techniques of this paper are not suitable for proving the desired completeness properties of the wave operators $W_\pm$ for the general class of exterior domains Ω considered in this section. For this reason, we now turn to a more restricted class of exterior domains, of considerable physical interest, for which these techniques do yield the completeness of $W_\pm$ in a physically very satisfactory sense.

III. SCATTERING BY PERIODIC SURFACES: MAIN RESULTS AND STRATEGY OF PROOF

The remaining sections of this paper will be devoted to scattering by periodic surfaces at which the homogeneous Dirichlet condition is imposed.

A. Statement of main results

Theorems 3.1 and 3.2 of this section are our principal results. Before stating them, some definitions are in order.

Let

$$L = \left\{ l \in \mathbb{R}^{\nu-1} : l = \sum_{i=1}^{\nu-1} n_i a_i, \ n_i \in \mathbb{Z}, \ i = 1,\ldots,\nu-1 \right\}, \tag{3.1}$$

where $\{a_i\}_{i=1}^{\nu-1}$ is a set of $\nu - 1$ linearly independent vectors in $\mathbb{R}^{\nu-1}$.

Henceforth, Ω will denote a domain in $\mathbb{R}^\nu$ $(\nu \geqslant 2)$ which satisfies Condition (I) of Sec. II and the additional condition

(II) (Periodicity) For all $l \in L$, $(\tilde{x},x_\nu) \in \Omega \Rightarrow (\tilde{x} + l, x_\nu) \in \Omega$.

As before, H will be defined by (2.1) and (2.2). Let

$\mathscr{H}_{\text{scatt}}(H)$, the subspace of scattering states of $\mathscr{H} = L^2(\Omega)$, and $\mathscr{H}_{\text{surf}}(H)$, the subspace of surface states of $\mathscr{H}$, be defined by

$$\mathscr{H}_{\text{scatt}}(H) = \left\{ f \in \mathscr{H} : \lim_{t \to \pm\infty} || \exp(-itH) f ||_{\Omega_a} = 0, \; 0 < a < \infty \right\}, \tag{3.2}$$

$$\mathscr{H}_{\text{surf}}(H) = \left\{ f \in \mathscr{H} : \lim_{a \to \infty} \sup_{t \in \mathbf{R}} || \exp(-itH) f ||_{\Omega \setminus \Omega_a} = 0 \right\}. \tag{3.3}$$

Here we have used the notation

$$A_a = \{(\tilde{x}, x_\nu) \in A : x_\nu < a\}. \tag{3.4}$$

It is easy to show that $\mathscr{H}_{\text{scatt}}(H)$ and $\mathscr{H}_{\text{surf}}(H)$ are closed linear manifolds of $\mathscr{H}$, i.e., that they are *subspaces* in the sense in which this word will always be used in this paper. One can also show that $\mathscr{H}_{\text{scatt}}(H)$ and $\mathscr{H}_{\text{surf}}(H)$ are mutually orthogonal (Lemma 8.1). Notice that $\mathscr{H}_{\text{scatt}}(H) \subset \mathscr{H}_{\text{ac}}(H)$, where $\mathscr{H}_{\text{ac}}(H)$ is the subspace of absolute continuity of $\mathscr{H}$ with respect to H. In general, one expects that this inclusion is proper, a point which has been forcefully made by Davies and Simon[2] in the context of a problem considered in the latter reference.

Theorem 3.1: The wave operators $W_\pm$ in (2.3) are complete, in the sense that

$$W_\pm^* W_\pm = E_\pm, \tag{3.5}$$

$$W_\pm W_\pm^* = P_{\text{scatt}}, \tag{3.6}$$

where $E_\pm$ and P_{scatt} are projection operators with domains $\mathscr{H}_0$, and $\mathscr{H}$, respectively, with $E_\pm \mathscr{H}_0 = \mathscr{H}_\pm$ [see (2.7)] and $P_{\text{scatt}} \mathscr{H} = \mathscr{H}_{\text{scatt}}$.

Theorem 3.2: Asymptotic completeness holds for $W_\pm$ in the sense that

$$\mathscr{H} = \mathscr{H}_{\text{scatt}}(H) \oplus \mathscr{H}_{\text{surf}}(H). \tag{3.7}$$

Remark: The way in which Theorems 3.1 and 3.2 have been stated suggests that they are true for a wider class of exterior domains than those considered in this section, not necessarily having any periodicity properties. An important problem for future research will be to extend Theorem 3.1 and 3.2 to such more general domains.

B. Method of proof

Some further definitions are needed before outlining our approach for proving Theorems 3.1 and 3.2.

Let

$$\omega^0 = G \times \mathbf{R}_+, \tag{3.8}$$

$$\omega = \Omega \cap \omega^0, \tag{3.9}$$

where G is given by

$$G = \left\{ y \in \mathbf{R}^{\nu-1} : y = \sum_{i=1}^{\nu-1} y^{(i)} a_i, \; y^{(i)} \in (0,1), \; i = 1,\ldots,\nu-1 \right\}, \tag{3.10}$$

and, hence, is an open periodicity cell of L in (3.1). By (3.8)–(3.10) and Property (I), $\omega \subset \omega^0$ and $\omega^0 \setminus \omega$ is bounded. Notice also that the closures of the union of all the translates of ω^0 and ω by the vectors of L equal Ω^0 [see (2.13)] and Ω, respectively.

Letting

$$\mathscr{G} = \left\{ \theta \in \mathbf{R}^{\nu-1} : \theta = \sum_{i=1}^{\nu-1} \theta^{(i)} b_i, \; \theta^{(i)} \in (0, 2\pi), \; i = 1,\ldots,\nu-1 \right\}, \tag{3.11}$$

where $\{b_i\}_{i=1}^{\nu-1}$ is a set of $\nu - 1$ linearly independent vectors in R such that $a_i \cdot b_j = \delta_{ij}$ $(i,j = 1,\ldots,\nu-1)$, we define the direct integrals

$$\mathscr{H}^0 = \int_{\mathscr{G}}^{\oplus} L^2(\omega^0) \, d\mu, \tag{3.12}$$

$$\mathscr{H}' = \int_{\mathscr{G}}^{\oplus} L^2(\omega) \, d\mu, \tag{3.13}$$

of Hilbert spaces, where $d\mu = |\mathscr{G}|^{-1} d\theta$, $d\theta$ being Lebesgue measure in $\mathbf{R}^{\nu-1}$ and $|\mathscr{G}|$ the Lebesgue measure of $\mathscr{G}$. We denote the "component" of a vector $k \in \mathscr{H}'$ in the θ th fiber $L^2(\omega)$ by k_θ.

We define unitary operators U^0 and U, with domains

$$\mathscr{H}^0 = L^2(\Omega^0)$$

and $\mathscr{H} = L^2(\Omega)$, respectively, and ranges $\mathscr{H}^0$ and $\mathscr{H}'$, respectively, where Ω^0 was defined in (2.13) [$\mathscr{H}^0$ should not be confused with $\mathscr{H}_0 = L^2(\mathbf{R}^\nu)$.] In particular, U is defined as follows. If $f \in L^2(\omega)$ is of bounded support,[18] then

$$(Uf)_\theta(x) = \sum_{l \in L} \exp(-il \cdot \theta) f(\tilde{x} + l, x_\nu), \quad \theta \in \mathscr{G}, \quad x = (\tilde{x}, x_\nu) \in \omega, \tag{3.14}$$

where only a finite number of summands in (3.14) are different from zero a.e. in ω. The set of all such f's is dense in $L^2(\omega)$, and it is easy to show, using (3.14) together with (3.1) and (3.11), that U, restricted to such f's is isometric:

$$||Uf||_{\mathscr{H}'}^2 = \int_{\mathscr{G}} ||(Uf)_\theta||_{L^2(\omega)}^2 \, d\mu = ||f||_{L^2(\Omega)}^2.$$

Therefore, U can be extended uniquely to the whole of $\mathscr{H}$ by continuity. One can prove that $U\mathscr{H} = \mathscr{H}'$, and hence that U is unitary. U^0 is defined in the same way as U, except with Ω and ω replaced by Ω^0 and ω^0, respectively.

In order to prove the desired completeness properties of $W_\pm(H, H_0)$, we introduce the self-adjoint operator

$$H^0 = -\Delta_D(\Omega^0), \tag{3.15}$$

where $\Delta_D(\Omega^0)$ is the Dirichlet Laplacian in H^0, acting by Δ on the functions in its domain, which is given by (2.2), but with Ω replaced by Ω^0. As is well known, H^0 has a purely absolutely continuous spectrum. In some vague sense, H is "intermediate" between H^0 and H_0 $(\Omega^0 \subset \Omega \subset \mathbf{R}^\nu)$. A crucial step here is to represent H^0 and H as direct integrals of operators:

$$U^0 H^0 (U^0)^{-1} = \int_{\mathscr{G}}^{\oplus} h_\theta^0 \, d\mu, \tag{3.16}$$

$$UHU^{-1} = \int_{\mathscr{G}}^{\oplus} h_\theta \, d\mu, \tag{3.17}$$

where h_θ^0 $(\theta \in \mathscr{G})$ and h_θ $(\theta \in \mathscr{G})$ are self-adjoint operators in $L^2(\omega^0)$ and $L^2(\omega)$, respectively, which will be completely characterized in Sec. III. Since the functions $\theta \mapsto h_\theta^0$ and $\theta \mapsto h_\theta$ from $\mathscr{G}$ (equipped with the measure μ) into the set of self-adjoint operators in $L^2(\omega^0)$ and $L^2(\omega)$, re-

spectively, are measurable, it follows that (3.12), (3.13), (3.16), and (3.17), as well as certain other expressions in this paper involving direct-integral decompositions, make sense. The measurability of $\theta \mapsto h_\theta$ is asserted by Lemma C.1, which is stated and proved in Appendix C. That of $\theta \mapsto h^0_\theta$ can be proved similarly. Equations (3.16) and (3.17) will be established in Sec. IV.

Our strategy for proving Theorems 3.1 and 3.2 will now be explained.

By the chain rule and Theorem 2.1(a),

$$W_\pm(H,H_0) = W_\pm(H,H^0;J^0)W_\pm(H^0,H_0;\mathscr{P}^0), \quad (3.18)$$

provided that the wave operators on the rhs of (3.18) exist. Here, J^0 is the restriction of J to $\mathscr{H}^0 = L^2(\Omega^0)$ and $\mathscr{H}^0$: $\mathscr{H}_0 \to \mathscr{H}^0$ is the extension of $\mathscr{P}$ given by

$$(\mathscr{P}^0 f)(x) = f(x), \quad f\in\mathscr{H}_0, \ x\in\Omega^0. \quad (3.19)$$

According to Lemma B.1 of Appendix B, $W_\pm(H^0,H_0;\mathscr{P}^0)$ exist, satisfy (3.5), and also satisfy (3.6) with P_{scatt} replaced by $I_{L^2(\Omega^0)}$. Hence, if Theorem 3.1 holds for $W_\pm(H,H^0;J^0)$, with the rhs of (3.5) modified to $I_{L^2(\Omega^0)}$, then this theorem holds for $W_\pm(H,H_0)$ in its original form. The first step in proving that $W_\pm(H,H^0;J^0)$ have this property is to show that the wave operators $W_\pm(h_\theta,h^0_\theta;\eta)$ $(\theta\in\mathscr{G})$ are partial isometries which are complete in the usual sense, η being the restriction of J^0 to $L^2(\omega^0)$. The properties that $\omega^0\setminus\omega$ is bounded and that in the present Dirichlet case ω automatically possesses the local compactness property (defined in subsection B of Sec. IV) for *every* bounded subset of $H^1(\omega)$ (Lemma 4.6) are both essential in our proof that $W_\pm(h_\theta h^0_\theta;\eta)$ are complete (Lemma 5.2). This proof is effected by invoking the previously mentioned variant[11] of results of Birman and Belopol'skii.[10] This completeness result leads to a variant of Theorem 3.1 in which P_{scatt} is replaced in (3.5) by the projection operator $P'_{ac}: \mathscr{H}\to\mathscr{H}$ defined by (5.3). The second, and final step is to show that $P'_{ac} = \mathscr{P}_{\text{scatt}}$. This is proved in Sec. VIII and is based in an essential way on the result (Lemma 7.6) that each h_θ $(\theta\in\mathscr{G})$ has an empty singular continuous spectrum.

This spectral result is also essential in our proof of Theorem 3.2. Given this result, the latter theorem follows directly from three elementary lemmas (Lemmas 8.1–8.3).

IV. SOME PROPERTIES OF THE OPERATORS h^0_θ, h_θ $(\theta\in\mathscr{G})$

Various function spaces, such as $H^1_{0,\text{loc}}(\bar\Omega)$, $L^2_{\text{loc}}(\Delta;\bar\omega)$, etc., and the corresponding inner products and norms will be used, mostly without comment, in this and the succeeding sections. Our notation for these spaces, which is partially similar to that of Wilcox[19] and Lyford,[5,6] is explained in Appendix A.

A. h^0_θ $(\theta\in\mathscr{G})$

Let

$$\mathscr{L} = \left\{\tau\in\mathbb{R}^{\nu-1}: \tau = 2\pi\sum_{i=1}^{\nu-1} n_i b_i, \ n_i\in\mathbb{Z}, \ i = 1,\ldots,\nu-1\right\}. \quad (4.1)$$

We also need to define

$$\tilde f_\tau(\xi,\theta) = L^2(\mathbb{R}_+)\text{-}\lim_{r\to\infty}\int_{\omega^0(r)} w_\tau(x;\xi,\theta) f(x)\, dx,$$

$$f\in L^2(\omega^0), \quad \text{a.e. } \xi\in\mathbb{R}_+, \quad \tau\in\mathscr{G}.$$

Here, we have used the notations (3.8) and

$$A(r) = \{x\in A: |x| < r\} \quad (4.2)$$

for an arbitarary subset $A\subset\mathbb{R}^\nu$. The $w_\tau(.;\xi,\theta)$'s are generalized eigenfunctions of $-\Delta$ in $L^2_{\text{loc}}(\Delta;\bar\omega^0)$ defined by

$$w_\tau(x;\xi,\theta) = (2/\pi|G|)^{1/2}\exp[i(\tau+\theta)\cdot\tilde x]\sin\xi x_\nu, \quad \tau\in\mathscr{L}, \ \xi\in\mathbb{R}_+, \ \theta\in\mathscr{G}, \quad (4.3)$$

and corresponding to the eigenvalue

$$\kappa_\tau(\xi,\theta) = \xi^2 + |\tau+\theta|^2, \quad (4.4)$$

where $|\cdot| = ||\cdot||_{\mathbb{R}^\nu}$, in this instance and $|G|$ denotes the Lebesgue measure of G [see (3.10)].

Lemma 4.1: Equation (3.16) holds, with h^0_θ $(\theta\in\mathscr{G})$ the self-adjoint operator with domain

$$D(h^0_\theta) = \left\{f\in L^2(\omega^0): \sum_{\tau\in\mathscr{L}}\int_0^\infty \kappa_\tau^2(\xi,\theta)|\tilde f_\tau(\xi,\theta)|^2\, d\xi < \infty\right\} \quad (4.5)$$

and action

$$h^0_\theta f(x) = -\Delta f(x) = L^2(\omega^0)\text{-}\lim_{p,r\to\infty}\sum_{|\tau|\le p}\int_{\omega^0(r)}\kappa_\tau(\xi,\theta)w_\tau(x;\xi,\theta)\tilde f_\tau(\xi,\theta)\, d\xi,$$
$$f\in D(h^0_\theta), \text{ a.e. } x\in\omega^0. \quad (4.6)$$

Remarks: (1) This is a well-known result.[20]

(2) h^0_θ can also be characterized in a manner similar to that in which h_θ is characterized in Lemma 4.4. The present characterization, (4.5) and (4.6), is more explicit and its consequence (4.7) will be used to prove Theorem 3.1.

(3) By standard arguments, Lemma 4.1 entails that the spectral measure $E(\cdot;h^0_\theta)$ for h^0_θ $(\theta\in\mathscr{G})$ is given by

$$(E(\delta;h^0_\theta)f)(x) = \sum_{\tau\in\mathscr{L}}\int_{\mathbb{R}_+}\chi_\delta(\kappa_\tau(\xi,\theta))w_\tau(x;\xi,\theta)\tilde f_\tau(\xi,\theta)\, d\xi, \quad \text{a.e. } x\in\omega^0, \quad (4.7)$$

provided that $\delta\subset\mathbb{R}$ is a bounded interval, χ_δ being the characteristic function of δ. Under this proviso, (4.7) makes sense, since only a finite number of the summands in (4.7) do not vanish for a.e. $x\in\omega^0$ and since each integrand on the rhs of (4.7), as a function of ξ, vanishes a.e. outside of a bounded subset of $\mathbb{R}_+$. It follows from (4.4) and (4.7) that the spectrum of h^0_θ $(\theta\in\mathscr{G})$ is absolutely continuous and consists of the closed interval $[\lambda(\theta),\infty)$, where

$$\lambda(\theta) = \min_{\tau\in\mathscr{L}}|\tau+\theta|^2, \quad \theta\in\mathscr{G}.$$

B. h_θ $(\theta\in\mathscr{G})$

Before defining the family $\{h_\theta,\theta\in\mathscr{G}\}$ of self-adjoint operators, we state the following:

Definition: A complex-valued function f on Ω is said to have Property (P_θ) for some $\theta\in\mathscr{G}$ if it is of the form

$$f(\tilde x,x_\nu) = \exp(i\theta\cdot\tilde x)u(\tilde x,x_\nu)$$

a.e. on Ω, where $u(\tilde x+l,x_\nu) = u(\tilde x,x_\nu)$ a.e. on Ω for all $l\in L$.

Let h_θ $(\theta\in\mathscr{G})$ be the operator in $L^2(\omega)$ with domain

$$D(h_\theta) = \{ f \in L^2(\Delta;\omega) \cap H^1(\omega) : f \text{ has an extension } \tilde{f} \in H^1_{0,\mathrm{loc}}(\bar{\Omega}) \text{ with Property } (P_\theta) \text{ and } \langle \nabla g, \nabla f \rangle_\omega = \langle g, -\Delta f \rangle_\omega,\ g \in D_\theta \} \tag{4.8}$$

and action

$$h_\theta f = -\Delta f,\ f \in D(h_\theta). \tag{4.9}$$

Here, for each $\theta \in \mathscr{S}$,

$$D_\theta = \{ f \in H^1(\omega) : f \text{ has an extension } \tilde{f} \in H^1_{0,\mathrm{loc}}(\bar{\Omega}) \text{ with Property } P_\theta \}. \tag{4.10}$$

For completeness, we remark that $D_\theta (\theta \in \mathscr{S})$ is the domain of a densely defined, closed, symmetric, and positive quadratic form, say q_θ:

$$q_\theta(g,f) = \langle \nabla g, \nabla f \rangle_\omega, \quad f,g \in D_\theta.$$

The unique self-adjoint operator associated with the form q_θ $(\theta \in \mathscr{S})$ is h_θ, whence $D_\theta = D(h_\theta^{\frac{1}{2}})$. None of these facts will be used here, except for the property that each q_θ is closed. This property is stated by the next lemma, and will play an important role in proving the self-adjointness of the h_θ's.

In Lemmas 4.2–4.4, we consider a fixed, but arbitrary $\theta \in \mathscr{S}$. In the proof of Lemma 4.2, as well as in many other arguments in this paper, the notation (4.2) will be used without comment.

Lemma 4.2: D_θ is a closed subspace of $H^1(\omega)$.

Proof: Let $\{f_n\} \subset D_\theta$ be a sequence converging to f in $H^1(\omega)$. Since by (4.10) each f_n has an extension $\tilde{f}_n = \exp(i\theta \cdot \tilde{x}) u_n$ to Ω which is in $H^1_{0,\mathrm{loc}}(\bar{\Omega})$, and has property (P_θ), it is easy to show that $\{\tilde{f}_n\}$ is Cauchy in $H^1_{0,\mathrm{loc}}(\bar{\Omega})$. Since $H^1_{0,\mathrm{loc}}(\bar{\Omega})$ is a (closed) subspace of $H^1_{\mathrm{loc}}(\bar{\Omega})$, it follows that $\tilde{f}_n \to g \in H^1_{0,\mathrm{loc}}(\bar{\Omega})$. Because of this and the assumption that $f_n \to f$ in $H^1(\omega)$, it follows that $g|\omega(r) = f|\omega(r)$ $(r \in \mathbb{R}_+)$, and hence that $g|\omega = f$.

It remains to prove that g has Property P_θ. This is deduced easily from the facts that each $\tilde{f}_n$ has this property and that $u_n \to u$ in $L^2_{\mathrm{loc}}(\bar{\Omega})$, where $u(\tilde{x} + l, x_\nu) = u(\tilde{x}, x_\nu)$ a.e. in Ω for all $l \in L$. ■

Lemma 4.3: h_θ is self-adjoint.

Proof: Since $C_0^\infty(\omega) \subset D(h_\theta)$, h_θ is densely defined. It follows from (4.8), (4.9), and the fact that $D(h_\theta) \subset D_\theta$ that

$$\langle g, h_\theta f \rangle_\omega = \langle \nabla g, \nabla f \rangle_\omega, \quad f,g \in D(h_\theta).$$

Hence, h_θ is symmetric, whence $h_\theta^* = h_\theta$ will follow[21] if there exists for each $g \in L^2(\omega)$ an element $u_g \in D(h_\theta)$ such that

$$(h_\theta + I_{L^2(\omega)}) u_g = g. \tag{4.11}$$

Now, D_θ is a (closed) subspace of the Hilbert space $H^1(\omega)$ by Lemma 4.2, and hence Riesz's representation theorem asserts that there exists for each $g \in L^2(\omega)$ a $u_g \in D_\theta$ such that

$$\langle v, u_g \rangle_{1,\omega} = \langle v, g \rangle_\omega, \quad v \in D_\theta, \tag{4.12}$$

where $\langle \cdot,\cdot \rangle_{1,\omega}$ is the inner product in $H^1(\omega)$. (Hereafter, we will use the inner product and norm notations of Appendix A without special comment.)

An argument similar to one of Wilcox[22] shows that u_g in (4.12) is in $L^2(\Delta;\omega)$ and that it also has the property

$$\Delta u_g = u_g - g, \tag{4.13}$$

so that (4.11) holds. Combining (4.12) with (4.13), we see that

$$\langle \nabla v, \nabla u_g \rangle_\omega = \langle v, -\Delta u_g \rangle_\omega, \quad v \in D_\theta,$$

whence $u_g \in D(h_\theta)$. ■

There is an alternative characterization of $D(h_\theta)$ which will be very useful in this paper.

Lemma 4.4: h_θ has domain

$$D(h_\theta) = \{ f \in L^2(\Delta;\omega) \cap H^1(\omega) : f \text{ has an extension } \tilde{f} \in L^2_{\mathrm{loc}}(\Delta;\bar{\Omega}) \cap H^1_{0,\mathrm{loc}}(\bar{\Omega}) \text{ with Property } (P_\theta) \}. \tag{4.14}$$

Remark: The intersection with $H^1(\omega)$ in the rhs of (4.14) is redundant, by Lemma 4.4, $D(h_\theta) \subset \mathscr{D}_\theta$ [see (4.14) and (7.1)], and an argument in the proof of Lemma 7.2. The same redundancy occurs in (4.8).

Proof of Lemma 4.4: Consider the set $D(h_\theta)$ defined by (4.8) and the set E_θ defined by the rhs of (4.14). Let $f \in D(h_\theta)$. Then the extension $\tilde{f}$ of f mentioned in (4.8) is in $L^2_{\mathrm{loc}}(\Delta;\bar{\Omega})$ by Lemma C.2 of Appendix C. Hence, $D(h_\theta) \subset E_\theta$. Now let $f \in E_\theta$. Then Lemma C.3 of that appendix asserts that (C9) holds for all $g \in D_\theta$. Therefore, $E_\theta \subset D(h_\theta)$ and, hence, $D(h_\theta) = E_\theta$. ■

We now establish the relation between H and the h_θ's stated in Sec. III.

Lemma 4.5: (3.17) holds.

Proof: Since each h_θ is self-adjoint and the function $\theta \mapsto h_\theta$ is measurable (Lemmas 4.3 and C.1), it follows that $\int_{\mathscr{S}}^{\oplus} h_\theta \, d\mu$ is self-adjoint. We will prove the present lemma by showing that the latter operator and UHU^{-1} coincide on a core of UHU^{-1}, namely on the set of all $g = Uf$ such that $f \in D(H)$ is of bounded support.

Let $g = Uf$ be of this type, so that each g_θ is given by the first line of (3.14). We will show that $g_\theta \in D(h_\theta)$, where now and henceforth in this proof we fix $\theta \in \mathscr{S}$. Clearly, $g_\theta \in L^2(\Delta;\omega) \cap H^1(\omega)$, since each function $f(\cdot + l, \cdot)$ in (3.14), restricted to ω, is in this intersection [as follows from $f \in D(H)$ and Property (II)] and in view of the property that only a finite number of the summands in (3.14) are not zero a.e. in ω. Extend g_θ to a function $\tilde{g}_\theta$ on Ω by the sum in (3.14). One sees easily that $\tilde{g}_\theta$ has Property (P_θ). In addition, one can show that $g_\theta \in L^2_{\mathrm{loc}}(\Delta;\bar{\Omega})$ by the same type of argument used to prove that $g_\theta \in L^2(\Delta;\omega)$.

We now prove that $\tilde{g}_\theta$ is also in $H^1_{0,\mathrm{loc}}(\bar{\Omega})$ and, hence, that $g_\theta \in D(h_\theta)$, by Lemma 4.4. Since $f \in H^1_0(\Omega)$ is of bounded support, there exists a sequence $\{f_n\} \subset C_0^\infty(\Omega)$ such that (a) supp f_n is contained for each n in an n-independent compact subset of $\mathbb{R}^\nu$ which also contains supp f and (b) $f_n \to f$ in $H^1(\Omega)$. Let

$$g_\theta^{(n,N)}(x) = \sum_{\substack{l \in L \\ |l| \le N}} \exp(-il \cdot \theta) f_n(\tilde{x} + l, x_\nu), \quad x = (\tilde{x}, x_\nu) \in \Omega,$$

for each n and all positive integers N. By (a), there exists for every $r \in \mathbb{R}_+$ a positive integer N_r such that $f(\tilde{x} + l, x_\nu) = f_n(\tilde{x} + l, x_\nu) = 0$ for a.e. $(\tilde{x}, x_\nu) \in \Omega(r)$ if $l \in L$ and $|l| > N_r$. Hence

$$\|\tilde{g}_\theta - g_\theta^{(n,N)}\|_{1,\Omega(r)} \le \sum_{\substack{l \in L, \\ |l| \le N}} \|f(\cdot + \cdot, \cdot) - f_n(\cdot + \cdot, \cdot)\|_{1,\Omega(r)} \to 0$$

for $n, N \to \infty$, $r \in \mathbb{R}_+$ $(\Omega(r) \neq \emptyset)$. (4.15)

By (4.15) and the fact that every $g_\theta^{(n,N)} \in C_0^\infty(\Omega)$, it follows that $g_\theta \in H^1_{0,\mathrm{loc}}(\bar{\Omega})$.

Using, among other properties, $g_\theta \in D(h_\theta)$, $f(\cdot + l, \cdot) \in D(H)$ $(l \in L)$, and the above finiteness property of the sum (3.14), we obtain

$$h_\theta g_\theta = -\Delta g_\theta = (U(-\Delta f))_\theta = (UHf)_\theta = (UHU^{-1}g)_\theta. \blacksquare$$

The property of local compactness which we now define will be of importance in future discussions.[23]

Definition: An open subset $A \subset \mathbb{R}^\nu$ will be said to have the local compactness (LC) property for a bounded subset $B \subset H^1(A)$ if B is precompact in $L^2(A(r))$ for all $r \in \mathbb{R}_+$, i.e., if for each such r each sequence $\{f_n\} \subset B$ has a subsequence $\{f_{n_k}\}$ which is independent of r and such that $\{f_{n_k} | L^2(A(r))\}$ is Cauchy in $L^2(A(r))$. (The equivalence of the two definitions is easily proved.)

Lemma 4.6: ω has the LC property for every bounded subset of $H^1(\omega)$ contained in D_θ $(\theta \in \mathscr{G})$.

Remarks: (1) In this paper, we will only apply this lemma to bounded subsets of $H^1(\omega)$ contained in $D(h_\theta) \subset D_\theta$ for some $\theta \in \mathscr{G}$.

(2) The fact that each $f \in D_\theta$ $(\theta \in \mathscr{G})$ has an extension to $H^1_{0,\mathrm{loc}}(\bar{\Omega})$ is essential in our proof of this lemma, because of our use of an ingenious argument of Lyford,[24] which is based on Rellich's theorem[25] in $\mathbb{R}^\nu$.

Proof of Lemma 4.6: For some $\theta \in \mathscr{G}$, let $\{g_n\}$ be a sequence in D_θ which is bounded in the $H^1(\omega)$-norm. By (4.10), each g_n has an extension $\tilde{g}_n \in H^1_{0,\mathrm{loc}}(\bar{\Omega})$. Let χ be the restriction to Ω of a function $X \in C_0^\infty(\mathbb{R}^\nu)$. Then $\chi \tilde{g}_n \in H^1_0(\Omega)$ for each n and hence can be identified in the usual way with a function in $H^1_0(\mathbb{R}^\nu)$. Therefore, by the above argument,[24] $\{\chi \tilde{g}_n | \Omega(r)\}$ is precompact in $L^2(\Omega(r))$ for each $r \in \mathbb{R}_+$. Since $X \in C_0^\infty(\mathbb{R}^\nu)$ is arbitrary, it follows that $\{\tilde{g}_n | \Omega(r)\}$, and hence $\{g_n | \omega(r)\}$, has this same precompactness property for every such r. $\blacksquare$

V. PROOF OF THEOREM 3.1

Let

$$W_\theta^\pm = W_\pm(h_\theta, h_\theta^0; \eta), \quad \theta \in \mathscr{G}, \tag{5.1}$$

$$W'_\pm = W_\pm(H, H^0; J^0), \tag{5.2}$$

where we remind the reader that H^0 was defined by (3.15) and that η and J^0 are the respective restrictions of J in (2.5) to $L^2(\omega^0)$ and $L^2(\Omega^0)$, respectively, where Ω^0 is as in (2.13). We also need to define the projection operator $P'_{\mathrm{ac}}: \mathscr{H} \to \mathscr{H}$, which is given by

$$UP'_{\mathrm{ac}}U^{-1} = \int_{\mathscr{G}}^{\oplus} P_{\mathrm{ac}}(h_\theta)\, d\mu, \tag{5.3}$$

where each $P_{\mathrm{ac}}(h_\theta)$ is the projection from $L^2(\omega)$ onto the subspace of absolute continuity of $L^2(\omega)$ with respect to h_θ.

Definition (5.3) makes sense because the function $\theta \to P_{\mathrm{ac}}(h_\theta)$ from $\mathscr{G}$ to $\mathscr{L}(L^2(\omega))$ is measurable, as follows from (5.5) (which holds by Lemma 5.2) and the fact that $\theta \to W_\theta^\pm$ are measurable functions, i.e., that $\theta \mapsto \langle g, W_\theta^\pm f \rangle_\omega$ are measurable functions for all $f \in L^2(\omega^0)$, $g \in L^2(\omega)$.[26] That $\theta \to W_\theta^\pm$ are measurable follows in a standard way from the corresponding property of $\theta \to h_\theta^0$ and $\theta \to h_\theta$ and the existence of $W_\theta^\pm$ $(\theta \in \mathscr{G})$ as strong limits.

Lemma 5.1: For each $\theta \in \mathscr{G}$, let $W_\theta^\pm$ exist and be partial isometries which are complete in the usual sense:

$$W_\theta^{*\pm} W_\theta^\pm = I_{L^2(\omega^0)}, \tag{5.4}$$

$$W_\theta^\pm W_\theta^{\pm *} = P_{\mathrm{ac}}(h_\theta). \tag{5.5}$$

Then $W'_\pm$ exist and are complete, in the sense that

$$W'^*_\pm W'_\pm = I_{L^2(\Omega^0)}, \tag{5.6}$$

$$W'_\pm W'^*_\pm = P'_{\mathrm{ac}}. \tag{5.7}$$

Proof: Combining (3.16) and (3.17) with (5.1), (5.2), and other pertinent definitions, one sees that $W'_\pm$ exist and that

$$UW'_\pm (U^0)^{-1} = \int_{\mathscr{G}}^{\oplus} W_\theta^\pm \, d\mu \tag{5.8}$$

under the assumptions of the lemma, where, of course, the direct integral in (5.8) denotes a bounded operator mapping each $g \in \mathscr{H}^{0\prime}$ [see (3.12)] into $k \in \mathscr{H}'$ [see (3.13)], with $k_\theta = W_\theta^\pm g_\theta$ for a.e. $\theta \in \mathscr{G}$. In particular, the facts that J and η are multiplication by C^∞ functions dependent only on x_ν is used to derive (5.8). The desired results (5.6) and (5.7) follow directly from (5.3)–(5.5) and (5.8). $\blacksquare$

Lemma 5.2. $W_\theta^\pm$ $(\theta \in \mathscr{G})$ have properties (5.4) and (5.5).

Remark: By Lemma 5.2 and the absolutely continuous nature of the spectrum of each h_θ^0, the absolutely continuous part of every h_θ is unitarily equivalent to h_θ^0. Hence, by Lemma 4.5, Remark (3) after Lemma 4.1, the fact that $H \geqslant 0$, and a standard argument, it follows that $\sigma(H) = [0, \infty)$. This result also follows, of course, by Lemmas 5.1 and 5.2, the well-known fact that H^0 has a purely absolutely continuous spectrum coinciding with $[0, \infty)$, and $H \geqslant 0$.

Before proving Lemma 5.2, we will use it to prove Theorem 3.1.

Proof of Theorem 3.1: Invoking, in particular, Lemmas 5.1 and 5.2, Lemma B.1 of Appendix B, and the consequence (3.18) of the chain rule, we see that the wave operators (2.3) exist, fulfill (3.5) and fulfill (3.6) with P_{scatt} replaced by P'_{ac}. The proof is completed by invoking (8.2), which is established in Sec. VIII. $\blacksquare$

Proof of Lemma 5.2: Since h_θ^0 has a purely absolutely continuous spectrum, this lemma will follow[11] if each of the properties (i)–(iii) below holds for all $\theta \in \mathscr{G}$ and all bounded intervals δ:

(i) $\eta D(h_\theta^0 \subset D(h_\theta)$, $\eta^*(h_\theta) \subset D h_\theta^0)$;

(ii) $(\eta^* - I_{L^2(\omega^0)})E(\delta; h_\theta^0)$ and $(\eta\eta^* I_{L^2(\omega)})E(\delta; h_\theta)$ are compact;

(iii) $(h_\theta \eta - \eta h_\theta^0)E(\delta; h_\theta^0)$ is trace class;

where $E(\cdot; h_\theta^0)$ and $E(\cdot; h_\theta)$ are the respective spectral measures for h_θ^0 and h_θ.

Henceforth in the proof, we consider a fixed $\theta \in \mathscr{G}$ and a fixed bounded interval $\delta \subset \mathbb{R}$. We proceed to show that (i)–(iii) hold for this θ and δ.

(i) We recall that the characterization of $D(h_\theta)$ in Lemma 4.4 applies to $D(h_\theta^0)$ if ω and Ω are replaced by ω^0 and Ω^0, respectively. Using, in particular, these characterizations, the definition of η, the assumption that the suppor

of $j \in C^\infty(\mathbb{R})$ lies in $[\frac{1}{2}, \infty)$, (3.8), (3.9), and Condition (I) of Sec. II, property (i) follows easily.

(ii) This property is provable by arguments of a well-known type,[27] so we will be brief. To prove the compactness of $(\eta\eta^* - I_{L^2(\omega)}) E(\delta; h_\theta)$ [that of $(\eta^*\eta - I_{L^2(\omega^0)}) E(\delta; h_\theta^0)$ can be proved similarly], it suffices to show that, for an arbitrary sequence $\{g_n\}$ which is bounded in $L^2(\omega)$, the sequence $\{u_n = E(\delta; h_\theta) g_n\}$, when restricted to $\omega(r)$, is precompact in $L^2(\omega(r))$ if $r \in \mathbb{R}_+$ is sufficiently large. This is because $\eta\eta^* - I_{L^2(\omega)}$ is multiplication by the function $(j^2 - 1)|_{\omega} \in C^\infty(\omega)$ of bounded support. Since each u_n is in $D(h_\theta) \subset D_\theta$, we find, by the "partial integration" property in (4.8), the spectral theorem and the boundedness of δ that $\{u_n\}$ is bounded in $H^1(\omega)$. Hence the desired precompactness property follows by Lemma 4.6.

(iii) Since only a finite number of terms on the rhs of (4.7) are nonvanishing for a.e. $x \in \omega^0$, and in view of the facts that the trace class is an ideal of the algebra of bounded operators and that for each τ the operator from $L^2(\omega^0)$ to $L^2(\mathbb{R}_+)$ defined by the map $f \to \tilde{f}_\tau(\cdot, \theta)$ is bounded, it suffices to show that for each τ the operator $T_{\tau,\theta}: L^2(\mathbb{R}_+) \to L^2(\omega)$ defined by

$$(T_{\tau,\theta} g)(x) = \int_{\mathbb{R}_+} \chi_\delta(\kappa_\tau)(\xi, \theta)) w_t(x; \xi, \theta)\, g(\xi)\, d\xi,$$

$$g \in L^2(\mathbb{R}_+), \text{a.e. } x \in \omega,$$

is trace class. This follows by applying an obvious variant of a well-known theorem of Stinespring.[28]

VI. POINT SPECTRUM OF h_θ $(\theta \in \mathscr{G})$

We know that the absolutely continuous spectrum of h_θ coincides with the spectrum of h_θ^0. (Recall the Remark after Lemma 5.2.) In this and the next section, we will discuss the singular spectrum of the h_θ's. The main result of the present section (Lemma 6.2) states, in particular, that the eigenvalues of each h_θ in suitable bounded intervals are of finite multiplicity and are isolated. This result will be applied in Sec. VII to prove that the singular continuous spectrum of every h_0 is empty.

In this section, $\theta \in \mathscr{G}$ will be fixed. This will allow us to simplify the notation by omitting θ from various symbols. For example, we write

$$k_\tau = |\tau + \theta|^2 \quad \tau \in \mathscr{L}, \tag{6.1}$$

where k_τ should not be confused with $\kappa_\tau(\xi, \theta)$ in (4.4) and where, we remind the reader, $\mathscr{L}$ was defined in (4.1).

For $f \in L^2_{\text{loc}}(\bar{\omega})$, we define

$$f_\tau(x_\nu) = \int_G \bar{\eta}_\tau(\tilde{x}) f(\tilde{x}, x_\nu)\, d\tilde{x}, \quad \tau \in \mathscr{L}, \text{ a.e. } x_\nu \in [1, \infty),$$

where G is as in (3.10) and

$$\eta_\tau(y) = |G|^{-\frac{1}{2}} \exp[i(\tau + \theta)\cdot y], \quad \tau \in \mathscr{L}, y \in \mathbb{R}^{\nu-1}. \tag{6.2}$$

Now, $\{\eta_\tau, \tau \in \mathscr{L}\}$ is a complete orthonormal set in $L^2(G)$ and

$$\omega_{a,\infty} = \{(\tilde{x}, x_\nu) \in \omega : x_\nu > a\}$$

is a purely cylindrical region for $a \geq 1$ by property (I) of Ω. Hence, we have for each $f \in L^2_{\text{loc}}(\bar{\omega})$,

$$f(x) = \sum_{\tau \in \mathscr{L}} \eta_\tau(\tilde{x}) f_\tau(x_\nu) \quad \text{a.e. } x \in \omega_{1,\infty}, \tag{6.3}$$

with the sum understood in the $L^2_{\text{loc}}(\bar{\omega}_{1,\infty})$ sense.

Lemma 6.1: Let f be an eigenfunction of h_θ pertaining to the eigenvalue λ:

$$h_\theta f = \lambda f.$$

Then

$$f(x) = \sum_{\substack{\tau \in \mathscr{L}, \\ k_\tau > \lambda}} C_\tau \exp\left(-\sqrt{k_\tau - \lambda}\, x_\nu\right) \eta_\tau(\tilde{x}), \quad \text{a.e. } x \in \omega_{1,\infty}$$

in the $L^2(\Delta; \omega_1)$ sense, where the C_τ's are constants.

Proof: Since $f \in D(h_\theta)$ by hypothesis, and since $D(h_\theta) \subset L^2(\omega)$ and $D(h_\theta) \subset \mathscr{D}_\theta$ [see (4.14) and (7.1)], this lemma is an immediate consequence of Lemma 7.3. ■

Lemma 6.2: Let I be an interval of the form $(-\infty, b]$ or $[a, b]$, where a, b are finite and where no k_τ's $(\tau \in \mathscr{L})$ are contained in $(-\infty, b)$ or $(a, b]$ in these two respective cases. Then h_θ has a finite number of eigenvalues in I and each such eigenvalue is of finite multiplicity.

Remarks: (a) Wilcox[29] has shown that the spectrum of h_θ is purely discrete when $\nu = 2$. His method of proof seems to be applicable to $\nu > 2$.

(b) Sufficient conditions for h_θ to have an empty point spectrum are known.[30]

Proof of Lemma 6.1: It will be by contradiction.[31] Let there exist an infinite sequence $\{\phi_m\}$ of orthonormal eigenfunctions of h_θ with eigenvalues in I. Since $\phi_m \in D(h_\theta) \subset D_\theta$ for each m, we have,

$$\|\nabla \phi_m\|_\omega^2 \leq b$$

for all m, so that $\{\phi_m\}$ is bounded in $H^1(\omega)$. Hence, by Lemma 4.6, $\{\phi_m\}$ has a subsequence, denoted henceforth by $\{\phi_m\}$, which is Cauchy in $L^2_{\text{loc}}(\bar{\omega})$.

Applying Lemma 6.1, we see that

$$\|\phi_m\|_{\omega_{r,\infty}} \leq \exp(-p(r-1)), r \in [1, \infty), m = 1, 2, \ldots, \tag{6.4}$$

where $p = \min\{(k_\tau - b)^{1/2}; k_\tau > b, \tau \in \mathscr{L}\}$ is positive by our assumptions on I. By (6.4) and the fact that $\{\phi_m\}$ is Cauchy in $L^2_{\text{loc}}(\bar{\omega})$, it follows that $\{\phi_m\}$ is also Cauchy in $L^2(\omega)$, which is impossible. ■

VII. ABSENCE OF THE SINGULAR CONTINUOUS SPECTRUM OF h_θ $(\theta \in \mathscr{G})$

A key ingredient in our proof of this fact is a result (Lemma 7.5) bounding $(h_\theta - \zeta)^{-1} f$ $(\theta \in \mathscr{G})$ for a set of f's dense in $L^2(\omega)$ as ζ tends to appropriate points on the real axis. Several lemmas needed to establish this result will be proved first.

We fix $\theta \in \mathscr{G}$ throughout this section, except in the remark after Lemma 7.6. Let

$$\mathscr{D}_\theta = \{f \in L^2_{\text{loc}}(\Delta; \bar{\omega}) \cap H^1_{\text{loc}}(\bar{\omega}) : f \text{ has an extension } \tilde{f} \in L^2_{\text{loc}}(\Delta; \bar{\Omega}) \cap H^1_{0,\text{loc}}(\bar{\Omega}) \text{ with Property } (P_\theta)\}. \tag{7.1}$$

The next two lemmas state properties of $\mathscr{D}_\theta$ which will be needed later in this section.

Lemma 7.1: If the sequence $\{f_n\} \subset \mathscr{D}_\theta$ is Cauchy in $L^2_{\text{loc}}(\Delta; \bar{\omega})$, then $f_n \to f \in \mathscr{D}_\theta$ in the $L^2_{\text{loc}}(\Delta; \bar{\omega})$ sense.

Proof: This follows by (7.1), Lemma C.4(a), and arguments similar to ones employed to prove Lemma 4.2. ■

Lemma 7.2: $\mathscr{D}_\theta \subset L^2(\Delta;\omega) = D(h_\theta)$.

Proof: By (7.1) and Lemma 4.4, $\mathscr{D}_\theta \cap L^2(\Delta;\omega) \cap H^1(\omega) = D(h_\theta)$. By (7.1) and Lemma (C.4)(a) [take $a \to \infty$ in (C.10)], $\mathscr{D}_\theta \cap L^2(\Delta;\omega) \cap H^1(\omega)$. ■

We will use the notation ω_a defined by (3.4), as well as the notation

$$\omega_{a,b} = \{(\tilde{x},x_\nu) \in \omega : a < x_\nu < b\}. \tag{7.2}$$

For $z \in \mathbb{C} \setminus (0,\infty)$, we define $\sqrt{z} = \sqrt{|z|}\exp(i\phi/2)$, with $\phi = \arg z \in (-\pi,\pi)$. For $z < 0$, it is immaterial for our purposes whether $\sqrt{z}$ is defined as $i\sqrt{|z|}$ or $-i\sqrt{|z|}$.

Lemma 7.3: (a) If $f \in \mathscr{D}_\theta$, then its expansion (6.3) is $L^2_{\mathrm{loc}}(\bar{\omega}_{1,\infty})$-convergent. If, in addition,

$$-\Delta f(x) = \zeta f(x)$$

a.e. in $\omega_{a,\infty}$ for some $a \in [1,\infty)$ and some $\zeta \in \mathbb{C}$, then the expansion "coefficients" of f in (6.3) are of the form

$$f_\tau(x_\nu) = C_\tau \exp(-\sqrt{k_\tau - \zeta}\, x_\nu) + D_\tau \exp(\sqrt{k_\tau - \zeta}\, x_\nu)$$

in $[a,\infty)$ for all $\tau \in \mathscr{L}$, where k_τ is as in (6.1) and C_τ and D_τ are constants.

Remark: Notice that $\mathrm{Re}\sqrt{k_\tau - \zeta} \geqslant 0$ for $\mathrm{Im}\,\zeta \neq 0$ and that $\mathrm{Im}\sqrt{k_\tau - \zeta} > 0$ (respectively, $\mathrm{Im}\sqrt{k_\tau - \zeta} < 0$) for $\mathrm{Im}\,\zeta < 0$ (respectively, $\mathrm{Im}\,\zeta > 0$).

Proof of Lemma 7.3: Since it follows by arguments similar to those used previously,[32] we will be brief. Let $f \in \mathscr{D}_\theta$. For each $b \in [a,\infty)$, let $\chi_b : L^2(\omega^0) \to L^2(\omega)$ be of the form $k_b \eta$, where $k_b : L^2(\omega) \to L^2(\omega)$ is multiplication by a $C^\infty(\mathbb{R})$ function which equals unity for $y \leqslant b$ and zero for $y \geqslant b + 1$. Here, $a \in [1,\infty)$. Considerations of the type used to prove property (i) in the proof of Lemma 5.2 show that $\chi_b^* f \in D(h_\theta^0)$ for each such b under the present assumptions. Using this result, together with (4.5)–(4.8), (6.1)–(6.3), Lemma 4.1, and the Fourier sine theorem,[33] and varying b over $[a,\infty)$, we find the expansion (6.3) of f converges in $L^2_{\mathrm{loc}}(\Delta;\omega_{1,\infty})$ and that each f_τ in this expansion has an absolutely continuous first derivative for $x_\nu \geqslant a$ and satisfies

$$\frac{d^2 f_\tau(x_\nu)}{dx_\nu^2} + (\zeta - k_\tau) f_\tau(x_\nu) = 0$$

a.e. in $[a,\infty)$. ■

Definition: $f \in L^2_{\mathrm{loc}}(\bar{\omega})$ is said to satisfy the outgoing (resp. incoming) radiation condition in ω if

$$f_\tau(x_\nu) \propto \begin{cases} \exp(-\sqrt{k_\tau - \lambda}\, x_\nu), & k_\tau \geqslant \lambda, \\ \exp(\pm i\sqrt{|k_\tau - \lambda|}\, x_\nu), & k_\tau < \lambda, \end{cases}$$

holds with the + (resp. −) sign for a.e. $x_\nu \in [a,\infty)$ for some $a \geqslant 1$, some $\lambda \in \mathbb{R}$, and all $\tau \in \mathscr{L}$.

Let

$$\Lambda = \{\lambda \in \mathbb{R} : \lambda \notin \sigma_p(h_\theta) \text{ and } \lambda \neq k_\tau,\ \tau \in \mathscr{L}\},$$

where $\sigma_p(h_\theta)$ is the point spectrum of h_θ.

Lemma 7.4 (*Uniqueness*): Let $f \in \mathscr{D}_\theta$ satisfy the incoming or outgoing radiation condition in ω and let $-\Delta f = \lambda f$ for some $\lambda \in \Lambda$. Then $f = 0$.

Proof: Let $f \in \mathscr{D}_\theta$ satisfy the outgoing radiation condition. (The case when f satisfies the ingoing radiation condition can be handled similarly.) By Lemma 7.3, there exists a set of constants $\{C_\tau, \tau \in \mathscr{L}\}$ such that

$$f(x) = \sum_{\tau \in \mathscr{L}} C_\tau \exp(\sigma_\tau \sqrt{|k_\tau - \lambda|}\, x_\nu)\eta_\tau(\tilde{x}) \tag{7.3}$$

in the $L^2_{\mathrm{loc}}(\Delta;\bar{\omega}_{a,\infty})$ sense, where a is some constant in $[1,\infty)$ and $\sigma_\tau = -1$, i in the respective cases $k_\tau > \lambda, k_\tau < \lambda$, the only possible cases since $\lambda \in \Lambda$. Invoking Lemma C.4 (b) of Appendix C, it follows that the series

$$\frac{\partial f(x)}{\partial x_\nu} = \sum_{\tau \in \mathscr{L}} C_\tau \sigma_\tau \sqrt{|k_\tau - \lambda|}\, \exp\left(\sigma_\tau \sqrt{|k_\tau - \lambda|}\, x_\nu\right)\eta_\tau(\tilde{x}), \tag{7.4}$$

obtained by formal differentiation of (7.3), is rigorously true in the sense of $L^2_{\mathrm{loc}}(\bar{\omega}_{a,\infty})$-convergence.

By $-\Delta f = \lambda f$, $f \in \mathscr{D}_\theta$, and Lemma C.5 of Appendix C, we conclude that

$$\int_G \left[\bar{f}\frac{\partial f}{\partial x_\nu} - f\frac{\partial \bar{f}}{\partial x_\nu}\right](\tilde{x},b)\, d\tilde{x} = 0 \tag{7.5}$$

for almost all $b \geqslant a$. [Actually, (7.5) holds for all $b > a$ by modifying f, if necessary, on a set of measure zero, since f, as the (weak) solution of the elliptic equation $-\Delta f = \lambda f$, is equivalent to a $C^\infty(\omega)$ function.] Using (7.3)–(7.5), we find in a very familiar way[34] that $C_\tau = 0$ for $k_\tau < \lambda$, whence $f \in L^2(\omega)$. Since $-\Delta f = \lambda f$, we see that $f \in L^2(\Delta;\omega)$. Applying Lemma 7.2, we infer that $f \in D(h_\theta)$. Since $\lambda \notin \sigma_p(h_\theta)$, the desired result $f = 0$ follows. ■

Let

$$R_\zeta = R_\zeta(h_\theta) = (h_\theta - \zeta)^{-1}$$

when ζ is in the resolvent set of h_θ.

Lemma 7.5: Let $(\gamma,\delta) \subset \Lambda$ be a bounded interval and let $a \in [1,\infty)$ be fixed. Then we have for all f in the unit ball of $L^2(\omega)$ with $\mathrm{supp}\, f \subset \omega_a$:

$$\|R_{\lambda \pm i\sigma} f\|_{1,\omega_b} \leqslant K_{a,b} \tag{7.6}$$

for all $b \in [a,\infty)$ $(\omega_b \neq \phi)$, provided that $\lambda \in (\gamma,\delta)$ and $\sigma \in (0,1)$. Here, $K_{a,b}$ is a constant independent of λ, σ, and f.

Remarks: Using this lemma together with standard arguments, one can show that a principle of limiting absorption holds for h_θ. In particular, it can be proved that the limits

$$L^2_{\mathrm{loc}}(\Delta;\bar{\omega})\text{-}\lim_{\sigma \downarrow 0} R_{\lambda \pm i\sigma}(h_\theta) f$$

exist for all the f's and λ's specified in Lemma 7.5. We will not need this result here.

Proof of Lemma 7.5: We will prove the lemma for the case of the + sign in (7.6). Suppose that the lemma is false in this case for *some* finite $b > a \geqslant 1$. (When the symbol b occurs hereafter in the proof, this b will always be meant.) Then there exist sequences $\{\zeta_n = \lambda_n + i\sigma_n\}$ and $\{f_n\}$, with $\lambda_n \in (\gamma,\delta)$, $\sigma_n \in (0,1)$, $\|f_n\|_{\omega_b} = 1$, and $\mathrm{supp}\, f_n \subset \omega_a$ for each n, such that

$$\|R_{\zeta_n} f_n\|_{1,\omega_b} \geqslant n$$

for all n. Since $(\gamma,\delta) \times (0,1)$ is a bounded region in $\mathbb{R}^2$, $\{\zeta_n\}$ will be assumed to converge without loss of generality. Hence, $\lambda_n \to \lambda \in (\gamma,\delta)$, since the lemma would be true otherwise.

For each n, let

$$u_n = ||R_{\zeta_n} f_n||_{1,\omega_b}^{-1} R_{\zeta_n} f_n, \quad g_n = ||R_{\zeta_n} f||_{1,\omega_b}^{-1} f_n,$$

whence $||u_n||_{1,\omega_b} = 1$ for all n and $g_n \to 0$ in $L^2(\omega)$ for $n \to \infty$.

Since $u_n \in D(h_\theta) \subset D_\theta$ for every n, it follows easily with the aid of Lemma 4.6 that $\{u_n\}$ has a subsequence, denoted by $\{u_n\}$ henceforth, which is Cauchy in $L^2(\omega_c)$ for each $c \in (0,b)$. Directly from the definitions, $-\Delta u_n = \zeta_n u_n + g_n$, so that $-\Delta u_n(x) = \zeta_n u_n(x)$ for a.e. $x \in \omega_{a,\infty}$ by the assumption that $\text{supp } f_n \subset \omega_a$. Taking also into account that $u_n \in L^2(\omega)$ for every n, we find by Lemma 7.3 that each u_n is given by an $L^2(\Delta;\omega_{1,\infty})$-convergent series (6.3), with $f_\tau(x_\nu)$ replaced by

$$(u_n)_\tau(x_\nu) = C_{n\tau} \exp(-\sqrt{k_\tau - \zeta_n}\, x_\nu), \quad \tau \in \mathscr{L}, \ x_\nu \in [a,\infty), \tag{7.7}$$

for some set $\{C_{n\tau}, \tau \in \mathscr{L}\}$ of constants. Whence $\|u_n\|_{\omega_{p,q}} \leqslant \|u_n\|_{\omega_{p,q}}$ for each n if $a \leqslant p \leqslant q < \infty$ and $0 \leqslant \rho < \infty$. Therefore, $\{u_n\}$ is Cauchy in $L^2_{\text{loc}}(\bar{\omega})$. Since $-\Delta u_n = \zeta_n u_n + g_n$, $\{u_n\}$ is Cauchy in $L^2_{\text{loc}}(\Delta;\bar{\omega})$ as well. Thus, $u_n \to u \in \mathscr{D}_\theta$ in $L^2_{\text{loc}}(\Delta;\bar{\omega})$, by Lemma 7.1, with

$$-\Delta u = \lambda u$$

for some $\lambda \in (\gamma,\delta)$. Using (7.7) in particular, one proves easily that u satisfies the outgoing radiation condition, whence $u = 0$ by Lemma 7.4.

However, since $u_n \to u$ in $L^2_{\text{loc}}(\Delta;\bar{\omega})$, Lemma C.4(a) entails that $u_n \to u$ in $H^1_{\text{loc}}(\bar{\omega})$. This result and the fact that $||u_n||_{1,\omega_b} = 1$ for all n implies that $u \neq 0$, a contradiction which proves the present lemma. ■

The principal result of this section is

Lemma 7.6: h_θ has an empty singular continuous spectrum.

Remark: By Lemma 7.6 and (3.17), H has a purely absolutely continuous spectrum if each h_θ has an empty point spectrum.

Proof of Lemma 7.6: Let $(\gamma,\delta) \subset \Lambda$ be a bounded interval and let $f \in L^2(\omega)$ be of bounded support. Then we find with the aid of Lemma 7.5 that

$$|\langle f, R_{\lambda \pm i\sigma} f\rangle_\omega| \leqslant \text{const}$$

for all pairs $(\lambda,\sigma) \in (\gamma,\delta) \times (0,1)$, where the constant is independent of λ and σ. Since the set of all such f's is dense in $L^2(\omega)$, it follows[36] that h_θ can have, at most, absolutely continuous spectrum in (γ,δ), i.e., that $\text{Ran}E((\gamma,\delta);h_\theta) \subset \mathscr{H}_{\text{ac}}(h_\theta)$. Using this result together with the fact, entailed by Lemma 6.2, that there exists a countable set of pairwise disjoint intervals whose interiors are in Λ and whose union equals $\mathbb{R}$, and with a simple limiting argument of a type used elsewhere,[37] the lemma follows. ■

VIII. PROOF OF THEOREM 3.2

Define the projection operator P_s with domain $\mathscr{H}$:

$$UP_sU^{-1} = \int_{\mathscr{G}}^{\oplus} P_p(\theta)\, d\mu.$$

As in Sec. V. $P_p(\theta)$ $(\theta \in \mathscr{G})$ is the projection from $L^2(\omega)$ onto the subspace $\mathscr{H}_p(h_\theta)$ of $L^2(\omega)$ which equals the closed span of the eigenfunctions of h_θ. As a by-product of results of this section, it will follow that

$$\text{Ran}\, P'_{\text{ac}} = \mathscr{H}_{\text{scatt}}(H), \tag{8.1}$$

$$\text{Ran}\, P_s = \mathscr{H}_{\text{surf}}(H), \tag{8.2}$$

where P'_{ac}, $\mathscr{H}_{\text{scatt}}(H)$, and $\mathscr{H}_{\text{surf}}(H)$ were defined in (5.3), (3.2), and (3.3), respectively.

In order to prove Theorem 3.2, we will need the next three simple lemmas.

Lemma 8.1: $\mathscr{H}_{\text{scatt}}(H)$ and $\mathscr{H}_{\text{surf}}(H)$ are mutually orthogonal subspaces of $\mathscr{H}$.

Proof: The subspace property follows by the usual argument, very familiar in the context of nonrelativistic scattering by short-range potentials.[38] If $0 \neq f \in \mathscr{H}_{\text{scatt}}(H)$, then for any $a \in \mathbb{R}_+$,

$$\sup_{t \in \mathbb{R}} ||\exp(-itH)f||_{\Omega \setminus \Omega_a} \geqslant \lim_{t \to \pm\infty} ||\exp(-tHf)||_{\Omega \setminus \Omega_a}$$
$$= ||f||_\Omega \neq 0,$$

where Ω_a was defined in (3.4). Thus, $f \notin \mathscr{H}_{\text{surf}}(H)$, whence the orthogonality property follows. ■

Lemma 8.2: $\text{Ran}P'_{\text{ac}} \subset \mathscr{H}_{\text{scatt}}(H)$.

Proof: Let $f \in \text{Ran}P'_{\text{ac}}$. Then $g = Uf$ has the property that $g_\theta \in \mathscr{H}_{\text{ac}}(h_\theta)$ for a.e. $\theta \in \mathscr{G}$. Consider a fixed θ for which this holds and a fixed $a \in [1,\infty)$. Letting $\chi(\omega_a)$ be multiplication in $L^2(\omega)$ by the characteristic function of ω_a, the operator $\chi(\omega_a)E(\delta;h_\theta)$ is compact for each bounded interval $\delta \subset \mathbb{R}_+$, as can be shown by means of an argument of the type used to prove property (ii) in the proof of Lemma 5.2. By Lemma 4.6 and a simple argument,[39] this compactness property entails that

$$\lim_{t \to \pm\infty} ||\exp(-ith_\theta) g_\theta||_{\omega_a} = 0,$$

where we used the notation (3.4).

Since

$$||\exp(-itH)f||^2_{\Omega_a} = \int_{\mathscr{G}}^{\oplus} ||\exp(-ith_\theta) g_\theta||^2_{\omega_a}\, d\mu$$

and

$$||\exp(-ith_\theta) g_\theta||_{\omega_a} \leqslant ||g_\theta||_\omega,$$

we conclude that

$$\lim_{t \to \pm\infty} ||\exp(-itH)f||_{\Omega_a} = 0,$$

by bounded convergence. ■

Lemma 8.3: $\text{Ran}P_s \subset \mathscr{H}_{\text{surf}}(H)$.

Proof: Similar to that of the corresponding result[40] of Ref. 2. ■

Proof of Theorem 3.2: By Lemma 7.6,

$$L^2(\omega) = \mathscr{H}_{\text{ac}}(h_\theta) \oplus \mathscr{H}_p(h_\theta), \quad \theta \in \mathscr{G}.$$

Combining this result with Lemmas 8.1–8.3, we see that

$$\mathscr{H} = \text{Ran}P'_{\text{ac}} \oplus \text{Ran}P_s$$
$$\subset \mathscr{H}_{\text{scatt}}(H) \oplus \mathscr{H}_{\text{surf}}(H), \tag{8.3}$$

whence (3.7) follows. ■

Equations (8.1) and (8.2) are immediate consequences of combining (8.3) with Lemmas 8.1–8.3.

ACKNOWLEDGMENTS

We are indebted to J. A. DeSanto for information about the theoretical literature of low-energy atomic-beam scattering by crystal surfaces and of classical scattering by periodic surfaces, as well as for helpful discussions. It is also a pleasure to thank C. Chandler and A. G. Gibson for penetrating comments on the investigations mentioned in Ref. 12, W. W. Zachary for many useful remarks, and C. I. Goldstein for a helpful letter. The author is grateful to P. Werner and C. H. Wilcox for their kind invitation to attend the Fourth Oberwolfach Conference on Scattering Theory, August 3–9, 1980, where the essential ideas of this paper were presented.

APPENDIX A: FUNCTION-SPACE NOTATION

Let A be an open subset of $\mathbb{R}^n$ $(n\geqslant 1)$. The norm and inner product in $L^2(A)$ will be written

$$\|\cdot\|_A,\ \langle\cdot,\cdot\rangle_A,$$

respectively. $L^2(\Delta;A)$ denotes the Hilbert space of all $f\in L^2(A)$ with $\Delta f\in L^2(A)$, equipped with the norm

$$\|f\|_{\Delta;A}=(\|f\|_A^2+\|\Delta f\|_A^2)^{\frac{1}{2}}.$$

The only Sobolev spaces $H_m(A)$ and $H_0^m(A)\subset H^m(A)$ used in this paper are $H^1(A)$ and $H_0^1(A)$. The norm and inner product in $H^1(A)$ are written as

$$\|f\|_{1,A}=\left(\|f\|_A^2+\sum_{i=1}^n\left\|\frac{\partial f}{\partial x_i}\right\|_A^2\right)^{\frac{1}{2}},$$

$$\langle g,f\rangle_{1,A}=\langle g,f\rangle_A+\sum_{i=1}^n\left\langle\frac{\partial g}{\partial x_i},\frac{\partial f}{\partial x_i}\right\rangle_A,$$

respectively. We will use the loose, but convenient notation

$$\langle\nabla g,\nabla f\rangle_A=\sum_{i=1}^n\left\langle\frac{\partial g}{\partial x_i},\frac{\partial f}{\partial x_i}\right\rangle_A.$$

$L^p_{\rm loc}(\bar{A})(p\geqslant 1)$ is the Fréchet space of (equivalence classes of) functions f on A with $f|A(r)\in L^p(A(r))$ $(r\in\mathbb{R}_+)$ and is equipped with a topology generated by the seminorms

$$\|\cdot\|_{A(r)},\quad r\in\mathbb{R}_+.$$

Here, $A(r)=\{x\in A:|x|<r\}$. $L^2_{\rm loc}(\Delta;\bar{A})$ is the Fréchet space of functions f on A with $f|A(r),\Delta f|A(r)\in L^2(A(r))$ $(r\in\mathbb{R}_+)$, whose topology is generated by the seminorms

$$\|\cdot\|_{L^p(A(r))},\quad r\in\mathbb{R}_+.$$

We also need $H^1_{\rm loc}(\bar{A})$, the Fréchet space composed of functions f on A with $f|A(r),\partial f/\partial x_i|A(r)\in L^2(A(r))$ $(r\in\mathbb{R}_+)$, its topology being generated by the seminorms

$$\|\cdot\|_{1,A(r)},\quad r\in\mathbb{R}_+.$$

Finally, $H^1_{0,\rm loc}(\bar{A})$ is a (closed) subspace of $H^1_{\rm loc}(\bar{A})$ obtained by completing $C_0^\infty(A)$ in the $H^1_{\rm loc}(\bar{A})$-topology.

In the symbols for the above Fréchet spaces, $\bar{A}$ has been used to indicate integrability up to the boundary.

APPENDIX B: SCATTERING BY AN IMPENETRABLE PLANE SURFACE

Although quantum scattering of a free particle by a plane surface with the homogeneous Dirichlet condition poses a very simple problem, explicit expressions for the relevant Møller wave operators are apparently not available in the accessible lieterature. We will state such expressions in this appendix and will use them to infer the desired properties of the wave operators in question.

As before, let H_0 and H^0 be defined by (2.1) and (3.15), respectively, where $\Omega^0=\mathbb{R}^{\nu-1}\times\mathbb{R}_+$, and write

$$W^0_\pm=W_\pm(H^0,H_0;\mathscr{P}^0)$$
$$=L^2(\Omega^0)-\lim_{t\to\pm\infty}\exp(itH^0)\mathscr{P}^0\exp(-itH_0),$$

where the operator $\mathscr{P}^0$: $\mathscr{H}_0=L^2(\mathbb{R}^\nu)\to L^2(\Omega^0)$ is defined by (3.19).

Lemma B.1: $W^0_\pm$ exist and are given by

$$(W^0_\pm f)(x)=\pm i\hat{f}_{\tilde{x}}(x_\nu),$$
$$f\in\mathscr{H}_0,\quad\text{a.e.}\quad x=(\tilde{x},x_\nu)\in\Omega^0,\tag{B1}$$

where for each $g:\Omega^0\to\mathbb{C}$, $g_{\tilde{x}}(\tilde{x}\in\mathbb{R}^{\nu-1})$ is the function on $\mathbb{R}_+$ with values $g_{\tilde{x}}(x_\nu)=g(\tilde{x},x_\nu)((\tilde{x},x_\nu)\in\Omega^0)$, and $\hat{}$ (resp. $\tilde{}$) is the Fourier (resp. sine Fourier) transform in $L^2(\mathbb{R})$ (resp. $L^2(\mathbb{R}_+)$).

Proof: It suffices to prove (B.1) when $f\in\mathscr{H}_0$ is of the form

$$f(\tilde{x},x_\nu)=f_1(\tilde{x})f_2(x_\nu),\tag{B2}$$

with $f_1\in L^2(\mathbb{R}^{\nu-1})$ and $f_2\in\mathscr{S}(\mathbb{R})$. In the respective representations where $L^2(\mathbb{R}^\nu)=L^2(\mathbb{R}^{\nu-1})\otimes L^2(\mathbb{R})$ and $L^2(\Omega^0)=L^2(\mathbb{R}^{\nu-1})\otimes L^2(\mathbb{R}_+)$, one has

$$\exp(itH_0)=\exp[-it\Delta(\mathbb{R}^{\nu-1})]\otimes\exp[-it\Delta(\mathbb{R})],\tag{B3}$$

$$\exp(itH^0)=\exp[-it\Delta(\mathbb{R}^{\nu-1})]\otimes\exp[-it\Delta_D(\mathbb{R}_+)],\tag{B4}$$

for $t\in\mathbb{R}$, where $\Delta(\mathbb{R}^{\nu-1})$, $\Delta\mathbb{R}$, and $\Delta_D(\mathbb{R}_+)$ are the Laplacian operators in $\mathbb{R}^{\nu-1}$, $\mathbb{R}$, and $\mathbb{R}_+$, respectively, the latter operator corresponding to a zero boundary condition at $0\in\mathbb{R}$. Using (B3), (B4), the fact that

$$[\exp(it\Delta_D(\mathbb{R}_+))g]\tilde{}(k)=\exp(-itk^2t)\tilde{g}(k),$$
$$g\in L^2(\mathbb{R}_+),\quad t\in\mathbb{R},\ \text{a.e. } k\in\mathbb{R}_+,$$

the one-dimensional form of (2.14), the pertinent definitions, and standard arguments, the first line of (B1) follows for f's of the form (B2). ■

Corollary: $W^0_\pm$ have the properties

$$W^0_\pm{}^*W^0_\pm=E_\pm,\tag{B5}$$

$$W^0_\pm W^0_\pm{}^*=I_{L^2(\Omega^0)},\tag{B6}$$

where $E_\pm$ are projections from $\mathscr{H}_0$ onto $\mathscr{H}_\pm$ [see (2.7)].

Proof: (B5) and (B6) follow immediately from (B1) using the unitarity of $\hat{}$ and $\tilde{}$. [Of course, (B5) is a special case of Theorem 2.1(b).] ■

APPENDIX C: MISCELLANEOUS LEMMAS

The principal purpose of this appendix is to state and prove five lemmas which are needed in Secs. III, IV, and VII.

Lemma C.1: The mapping

$$\theta\to H_\theta\tag{C1}$$

from $\mathscr{G}$ into the set of self-adjoint operators in $L^2(\omega)$ is measurable, i.e., $\langle g,(h+i)^{-1}f\rangle_\omega:\mathscr{G}\to\mathbb{C}$ is measurable for all f, $g\in L^2(\omega)$.

Proof: Consider the mapping

$$\theta\to h'_\theta=\exp(-\theta\cdot\tilde{x})h_\theta\exp(i\theta\cdot\tilde{x})\tag{C2}$$

from $\mathscr{G}$ into the set of self-adjoint operators in $L^2(\omega)$, where $\exp(\pm i\theta\cdot\tilde{x})$ denotes multiplication by the corresponding functions. For the present purpose, the advantage of the mapping (C2) over (C1) is that the domain of h'_θ $(\theta\in\mathscr{G})$, say D, is independent of θ. One readily shows that $D = D(h_0)$, the set defined by (4.8) for $\theta = 0$, and that

$$h'_\theta f = (-\Delta + w_\theta) f, \quad \theta\in\mathscr{G}, \quad f\in D, \tag{C3}$$

where $w_\theta = 2i\sum_{j=1}^{\nu-1}\theta_j(\partial/\partial x_j) + |\theta|^2$.

Using (C3) and the easily provable fact that w_θ is h_θ-bounded for each $\theta\in\mathscr{G}$, one readily shows that $\langle g,(h'_\theta + i)^{-1} f\rangle_\omega : \mathscr{G}\to\mathbb{C}$ is continuous, and even real-analytic, and hence that (C2) is measurable. Since $h'_\theta = \exp(i\theta\cdot\tilde{x}) h_\theta \exp(-i\theta\cdot\tilde{x})$ $(\theta\in\mathscr{G})$ and since the mappings $\theta\to\exp(\pm i\theta\cdot\tilde{x})$ from $\mathscr{G}$ into $\mathscr{L}(L^2(\omega))$ are measurable, it therefore follows that (C1) is measurable. ■

Lemmas C.2–C.5 and the Corollary to Lemma C.3 below refer to an arbitrary, but fixed $\theta\in\mathscr{G}$. In these lemmas, the definitions (4.10) of D_θ and (7.1) of D_θ should be kept in mind. In this appendix, the symbol $D(h_\theta)$ is only needed in the statement and proof of Lemma C.2, where it should be understood in the sense of (4.8). *The alternative characterization* (4.14) *of* $D(h_\theta)$ *is not used in this appendix.* Indeed, Lemma C.2 is used in Sec. IV to prove (4.14).

Lemma C.2: Let $f\in D(h_\theta)$ and let $\tilde{f}$ be the extension of f defined by (4.8). Then $\tilde{f}\in L^2_{\mathrm{loc}}(\Delta;\bar{\Omega})$.

Proof: It suffices to show that $\Delta\tilde{f}$ exists and is in $L^2_{\mathrm{loc}}(\Delta;\bar{\Omega})$. We will show this by proving that

$$\langle f,\Delta\phi\rangle_\Omega = \langle g,\phi\rangle_\Omega \tag{C4}$$

for all $\phi\in C_0^\infty(\Omega)$, where g is the function on Ω whose restriction to the translate ω_l of ω by each $l\in L$ [see (3.1)] equals $\Delta(\tilde{f}|\omega_l) = \Delta f^{(l)}\in L^2(\omega)$. In this proof, if $k\in L^2(\Omega)$, we denote by $k^{(l)}$ $(l\in L)$ a function with values $k^{(l)}(\tilde{x},x_\nu) = k(\tilde{x}+l,x_\nu)$ for $(\tilde{x},x_\nu)\in\omega$. This definition of g is legitimate, since, for each $l\in L$, $\tilde{f}|\omega_l\in L^2(\Delta;\omega_l)$ and $\Delta(\tilde{f}|\omega_l) = \exp(il\cdot\theta)\Delta f(\cdot - l,\cdot)$.

Define $\psi\in C^\infty(\omega)$ by

$$\psi = \sum_{l\in L}\exp(-il\cdot\theta)\phi^{(l)}, \tag{C5}$$

whence $\psi\in D_\theta$. Since $f\in D(h_\theta)$, we therefore conclude by (4.8) that

$$\langle\nabla\psi,\nabla f\rangle_\omega = \langle\psi,-\Delta f\rangle_\omega. \tag{C6}$$

Using the above expression for $\Delta(\tilde{f}|\omega_l)$ and (C5), we have

$$\begin{aligned}\langle g,\phi\rangle_\Omega &= \sum_{l\in L}\langle g,\phi\rangle_{\omega_l}\\ &= \sum_{l\in L}\int_\omega \exp(-il\cdot\theta)\Delta\tilde{f}(\tilde{x},x_\nu)\phi(\tilde{x}+l,x_\nu)\,dx\\ &= \langle\Delta f,\psi\rangle_\omega.\end{aligned} \tag{C7}$$

Similarly,

$$\langle\tilde{f},\Delta\phi\rangle_\Omega = -\langle\nabla f,\nabla\psi\rangle_\omega. \tag{C8}$$

Equations (C4) now follows from (C6)–(C8). ■

Lemma C.3: Let $f\in E_\theta = \{k\in L^2(\Delta;\omega)\cap H^1(\omega)$: k has an extension $\tilde{k}\in L^2_{\mathrm{loc}}(\Delta;\bar{\Omega})\cap H^1_{0,\mathrm{loc}}(\bar{\Omega})$ with Property $(P_\theta)\}$ and let $g\in D_\theta$. Then

$$\langle\nabla g,\nabla f\rangle_\omega = \langle g,-\Delta f\rangle_\omega. \tag{C9}$$

Proof: Analogous, but notationally more complicated, than the proof of a parallel result of Ref. 6.[41] ■

Corollary: Let $f\in\mathscr{D}_\theta$ and $g\in D_\theta$, and let g have bounded support. Then (C9) holds.

Proof: Let supp $g\subset\omega_a$ for some $0<a<\infty$, where ω_a is as in (3.4). Let χ be the restriction to ω of a $C^\infty(\mathbb{R}^\nu)$ function which depends only on $x_\nu\leqslant b$, and vanishes for $x_\nu\geqslant b+1$, for some finite $b\geqslant a$. Then $f\chi\in E_\theta$ by arguments of the same type as those used to prove Lemma 4.2. The present corollary now follows easily by applying (C9) with f replaced by χf. ■

In the next lemma, we use the notations (3.4) and (7.2).

Lemma C.4: Let $f\in\mathscr{D}_\theta$.

(a) If $1\leqslant a<\infty$ and $0<r<\infty$, then

$$||f||^2_{1,\omega_a}\leqslant(2+\pi/r^2)||f||^2_{\omega_{a+r}} + ||\Delta f||^2_{\omega_{a+r}}. \tag{C10}$$

(b) If $1\leqslant a<b<\infty$ and $0<r<\infty$, then (C10) holds with ω_a and ω_{a+r} replaced by $\omega_{a,b}$ and $\omega_{a-r,b-r}$, respectively.

Proof: Since it is similar to the proof of a parallel result in Ref. 35,[42] we will be brief. Only the proof of (a) will be sketched; (b) can be proved by arguments of the same character.

Let $f\in\mathscr{D}_\theta$ and let $\rho\in C^1(\omega)$ be defined by

$$\rho(\tilde{x},x_\nu) = \begin{cases} 1, & x_\nu<a,\\ \sin^2[\pi(a+r-x_\nu)/2r], & a\leqslant x_\nu\leqslant a+r,\\ 0, & x_\nu>a+r,\end{cases} \quad (\tilde{x},x_\nu)\in\omega, \tag{C11}$$

with a and r as in (a). One easily proves that $\rho f\in D_\theta$. Consequently, we have by applying the last corollary:

$$\begin{aligned}||\nabla f||^2_{\omega_a} &\leqslant \langle\rho\nabla f,\nabla f\rangle_\omega \leqslant |\langle\nabla(\rho f),\nabla f\rangle_\omega| + |\langle f\nabla\rho,\nabla f\rangle_\omega|\\ &= |\langle\rho f,\Delta f\rangle_\omega| + |\langle f\nabla\rho,\nabla f\rangle_\omega|.\end{aligned} \tag{C12}$$

Using (C11) and (C12) together with Schwarz's inequality, the elementary inequality

$$\alpha\beta\leqslant(1/2\delta)\alpha^2 + (\delta/2)\beta^2, \quad 0\leqslant\alpha,\beta<\infty, \quad 0<\delta<\infty,$$

and $0\leqslant\rho(x)\leqslant 1$ and $|\partial\rho(x)/\partial x_\nu|\leqslant(\pi/r)\rho^{\frac{1}{2}}(x)$ $(x\in\omega)$, we obtain (C10). ■

Lemma C.5: Let $f, g\in\mathscr{D}_\theta$. Then

$$\begin{aligned}&\int_{\omega_a}(\bar{g}\Delta f - f\Delta\bar{g})(\tilde{x},x_\nu)\,dx\\ &\quad = -\int_G\left(\bar{g}\frac{\partial f}{\partial x_\nu} - f\frac{\partial\bar{g}}{\partial x_\nu}\right)(\tilde{x},a)\,d\tilde{x}, \quad \text{a.e. } a\in[1,\infty).\end{aligned} \tag{C13}$$

Proof: Let $\{\Phi_n\}_{n=1}^\infty\subset C^\infty(\omega)$ be a sequence of functions having the form

$$\Phi_n(x) = -\sigma(x_\nu)W_n(x_\nu), \quad x = (\tilde{x},x_\nu)\in\omega, \tag{C14}$$

for each n, where

$$W_n(y) = \frac{1}{\pi}\int_{n(y-a)}^\infty \exp(-u^2)\,du, \quad y\in\mathbb{R}, \tag{C15}$$

and where $\sigma\in C^\infty(\mathbb{R})$ is such that

$$\sigma(y) = \begin{cases}1, & y\leqslant b,\\ 0, & b+1\leqslant y<\infty,\end{cases} \tag{C16}$$

for some finite $b > a$. One readily shows that $\Phi_n f$, $\Phi_n g \in \mathscr{D}_\theta$ for each n, and hence that

$$\int_\omega \Phi_n(\bar{g}\Delta f - f\Delta\bar{g})\, dx$$

$$= -\int_\omega [\nabla(\Phi_n\bar{g})\cdot\nabla f - \nabla(\Phi_n f)\cdot\nabla\bar{g}]\, dx$$

$$= -\int_\omega \frac{\partial\Phi_n}{\partial x_\nu}\left(\bar{g}\frac{\partial f}{\partial x_\nu} - f\frac{\partial\bar{g}}{\partial x_\nu}\right) dx, \tag{C17}$$

where we have used the Corollary to Lemma C.3.

Using (C.14)–(C.16) and a classical theorem on the Weierstrass singular integral,[43] it follows that

$$\lim_{n\to\infty}\int_{\mathbb{R}} \frac{\partial\Phi_n(\tilde{x},x_\nu)}{\partial x_\nu} F(x_\nu)\, dx_\nu = F(a), \tag{C18}$$

$$\lim_{n\to\infty}\int_\omega \Phi_n(\tilde{x},x_\nu)G(\tilde{x},x_\nu)\, dx = \int_{\omega_a} G(\tilde{x},x_\nu)\, dx, \tag{C19}$$

for a.e. $a \in [1,\infty)$ if $F \in L^1_{\mathrm{loc}}(\mathbb{R})$ and $G \in L^1_{\mathrm{loc}}(\bar{\omega})$. Applying (C18) and (C19) with

$$F(x_\nu) = \begin{cases} \displaystyle\int_G \left(\bar{g}\frac{\partial f}{\partial x_\nu} - f\frac{\partial\bar{g}}{\partial x_\nu}\right)(\tilde{x},x_\nu)d\tilde{x}, & x_\nu \geqslant 1, \ \text{a.e.}\, x_\nu \in [1,\infty), \\ 0, & \text{a.e.}\, x_\nu \in (\infty,1), \end{cases}$$

$$G(\tilde{x},x_\nu) = (\bar{g}\Delta f - f\Delta\bar{g})(\tilde{x},x_\nu), \quad (\tilde{x},x_\nu)\in\omega,$$

and using (C17) and Fubini's theorem, (C13) follows. ■

[1]See, e.g., G. Boato, P. Cantini, U. Garibaldi, A. C. Levi, L. Mattera, R. Spadacini, and G. E. Tommei, J. Phys. C: Solid State Phys. **6**, L394 (1973); R. L. Masel and R. P. Merrill, Phys. Rev. B **12**, 5545 (1975); F. O. Goodman, J. Chem. Phys. **68**, 976 (1977); N. García and N. Cabrera, Phys. Rev. B **18**, 576 (1978).

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[6]W. C. Lyford, Math. Ann. **236**, 255 (1978).

[7]See, e.g., Ref. 8, Sec. XIII.16 and Notes to Sec. XIII.16. See also Ref. 2.

[8]M. Reed and B. Simon, *Methods of Modern Mathematical Physics IV: Analysis of Operators* (Academic, New York, 1978).

[9]See, e.g., M.Reed and B. Simon, *Methods of Modern Mathematical Physics III: Scattering Theory* (Academic, New York, 1979), p. 35.

[10]M. Sh. Birman, Izv. Akad. Nauk SSSR, Ser. Mat. **32**, 914 (1968) [Math. USSR Izv. **2**, 879 (1968)]; A. L. Belopol'skii and M. Sh. Birman, Izv. Akad. Nauk SSSR, Ser. Mat. **32**, 1162 (1968) [Math. USSR Izv. **2**, 1117 (1968)].

[11]Ref. 5, Theorem 3.2.[12]

[12]This theorem of Lyford follows directly from Theorem 2.2.6 of P.A. Deift, "Classical Scattering with a Trace Condition," Ph. D. thesis, Princeton University, 1976. The latter theorem [essentially due to W. C. Lyford, Math. Ann. **217**, 257 (1975); Erratum: Math. Ann. **229**, 96 (1977)] was obtained by Deift as a by-product of the illuminating redevelopment of the Kato–Birman–Belopol'skii theory which he carried out in his thesis. In particular, a key role in this redevelopment is played by the generalized Birman trace theorem proved by D. B. Pearson, J. Functional Anal. **28**, 182 (1978).

[13]C. H. Wilcox, "Scattering Theory for Diffraction Gratings," Preprint 406, University of Bonn, 1980.

[14]C. H. Wilcox, "Rayleigh-Bloch Expansions for Diffraction Gratings, I and II," Preprints 363 and 407, University of Bonn, 1980.

[15]All derivatives in this paper should be understood in the distributional sense.

[16]This can be proved in several ways. For example, it follows by applying an obvious modification of Lemma 1.2 of E. B. Davies, Math. Proc. Camb. Phil. Soc. **82**, 327 (1977) appropriate to the space $L^2(\mathbb{R})$.

[17]See, e.g., M. Reed and B. Simon, *Methods of Modern Mathematical Physics II: Fourier Analysis, Self-Adjointness* (Academic, New York, 1975), p. 60, Theorem IX.31.

[18]If $f \in L^2(A)$ where A is an open subset of $\mathbb{R}^\nu$, the support of f is the complement in A of the largest open set $B \subset A$ such that $\|f\|_B = 0$.

[19]C. H. Wilcox, *Scattering Theory for the d'Alembert Equation in Exterior Domains*, Lecture Notes in Mathematics **442** (Springer, New York, 1975).

[20]It is provable by arguments differing only in notation from, e.g., those in Sec. 2 of Ref. 5.

[21]See, e.g., K. Yoshida, *Functional Analysis* (Springer, New York, 1966), Corollary, p. 199.

[22]Ref. 19, pp. 43, 44.

[23]A similar definition is given in Ref. 19, p. 60.

[24]Ref. 6, proof of Theorem 1.5.

[25]S. Agmon, *Lectures on Elliptic Boundary Value Problems* (Van Nostrand, Princeton, N.J., 1965), Theorem 3.8, p. 30.

[26]The measurability of $\theta \mapsto P_{\mathrm{ac}}(h_\theta)$ also follows by the result $P_{\mathrm{ac}}(h_\theta) = I_{L^2(\omega)} - P_p(h_\theta)$ $(\theta \in \mathscr{G})$, entailed by Lemma 7.6, and the measurability of $\theta \to P_p(h_\theta)$ (see Ref. 2, Proposition 2.2.2). Here, each $P_p(h_\theta)$ is the projection from $L^2(\omega)$ onto the closed span of the eigenfunctions of h_θ.

[27]See, e.g., Ref. 19, pp. 175, 176.

[28]W. F. Stinespring, J. Reine Angew. Math. **200**, 200 (1958), Theorem 2.

[29]Ref. 14, I, Corollary 4.12, p. 42.

[30]See, e.g., Ref. 14, I Theorem 2.2, p. 19. This theorem is essentially due to H. D. Alber, Proc. Roy. Soc. Edinburgh **82A**, 251 (1979).

[31]This proof is similar to that of Theorem 6.4, pp. 56–58, Ref. 4.

[32]See, e.g., Ref. 5, Sec. 2 and the first Appendix.

[33]See, e.g., N. Dunford and J. T. Schwartz, *Linear Operators* (Interscience, New York, 1963), Part II, p. 1388.

[34]Ref. 35, pp. 181, 182.

[35]D. M. Eidus, Am. Math. Soc. Trans. **47**, 157 (1965).

[36]Ref. 8, Theorem XIII.20, p. 138.

[37]See, e.g., J. R. Schulenberger and C. H. Wilcox, Arch. Rational Mech. Anal. **41**, 46 (1971), proof of Theorem 4.1.

[38]See, e.g., W. O. Amrein, J. M. Jauch, and K. B. Sinha, *Scattering Theory in Quantum Mechanics* (Benjamin, Reading, Mass., 1977), proof of Proposition 7.1, p. 263.

[39]Ref. 5, proof of Lemma 1.6.

[40]Ref. 2, proof of Proposition 6.1.

[41]Ref. 6, proof of Lemma 2.1.

[42]Ref. 35, proof of Lemma 1, pp. 159, 160.

[43]See, e.g., E. C. Titchmarsh, *Introduction to the Theory of Fourier Integrals* (Clarendon, Oxford, 1948), 2nd ed., Theorem 16, p. 31.

Radiative degrees of freedom of the gravitational field in exact general relativity

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(Received 24 March 1981; accepted for publication 22 May 1981)

The radiative degrees of freedom of the gravitational field are isolated by analyzing the structure available at null infinity, $\mathscr{I}$. It is shown thay they are coded in certain equivalence classes $\{D\}$ of connections; all information about gravitational radiation can be extracted from the curvature tensors of these connections directly on $\mathscr{I}$, without any reference to the interior of space–time. The space of classical vacua—i.e., of $\{D\}$ with trivial curvature—is analyzed. It is shown that the quotient ST/T of the BMS supertranslation group by its translation subgroup acts simply and transitively on this space. The available structure is compared with that of gauge theories. Since the entire discussion can be carried out on $\mathscr{I}$, without any reference to the interior, it suggests a new approach to quantum gravity. This approach will be presented in detail in a subsequent paper.

PACS numbers: 04.20.Cu, 04.60. + n, 04.30. + n

I. INTRODUCTION

This is the first of two papers whose goal is to suggest a new approach to quantum gravity. The general ideas underlying this approach were briefly summarized elsewhere.[1] Our purpose here is to provide a complete description. This include the proofs of the results quoted in Ref. 1 as well as of new results obtained since that presentation.

Traditional attempts at obtaining a quantum theory of gravity may be divided into two broad classes[2]: "covariant" approaches and "canonical" methods. In the first approach, one treats gravity in the spirit of other field theories and focuses on scattering processes involving gravitons, while, in the second, one emphasizes the geometrical nature of the gravitational field and attempts quantization via Hamiltonian methods. Both avenues have led to a number of insights. However, they also have obvious limitations. In the covariant approach, for example, one begins by splitting the dual role played by the space–time metric g_{ab}, in general relativity: One introduces a background metric η_{ab}, usually chosen to be flat, which is to provide the "kinematic arena," and regards $h_{ab} = g_{ab} - \eta_{ab}$ as the dynamical field. Thus, the geometrical role of g_{ab} is assigned to η_{ab}, while the role of the gravitational potential is now played by h_{ab}. Einstein's equation on g_{ab} provides a nonlinear field equation on h_{ab}. One first linearizes this equation and subjects the linear field to quantization following the usual rules of Minkowskian field theories. The resulting quanta are called gravitons. These are *then* subject to interactions dictated by the original nonlinear equation. While this procedure may seem to be a natural one from the field-theoretic viewpoint, it appears to be rather artificial from the standpoint of general relativity. For the dual role of the metric is a most essential feature of Einstein's theory and splitting of these roles violates the very spirit of the theory. Thus, it is unsettling to see the fictitious background η_{ab} play a significant role in the resulting theory: Notions such as the microcausality of field operators, asymptotoic regions for in and out states, spin and mass of the particles involved, all refer η_{ab}. Indeed, the very name "covariant" refers to the Poincaré covariance with respect to this flat background. Secondly, the fact that an essential use of the linearization procedure is made in the introduction of the basic notion of a graviton is also unappealing.[3] Even if such aesthetic considerations are ignored, one is still faced with significant difficulties. These arise from the fact that, since the underlying manifold structure is required to be $\mathbb{R}^4$, one cannot hope to encompass processes involving nontrivial topologies such as the formation and evaporation of a black hole. And, presumably, it is precisely through such qualitatively new processes that quantum gravity will make its impact felt. Indeed, the detailed numerical predictions for scattering processes which have played a key role in the development of other field theories seem, at the moment, uninteresting in the gravitational case, given the weakness of the coupling constant. The issues of immediate interest are, rather, the conceptual ones. And, it appears that covariant approaches avoid these very issues by imitating Minkowskian quantum field theories. Canonical methods, on the other hand, are better equipped to handle these questions. For, the emphasis is now on understanding, already at the classical level, ways in which general relativity differs from other field theories due to the geometrical nature of the gravitational field. Here, one neither introduces a background metric nor a linearization of Einstein's equation. The first step in the program is to cast exact general relativity in the Hamiltonian form. This was achieved a number of years ago and has shed much light on the geometrical significance of the constraints which must be satisfied by initial data on a spacelike Cauchy surface. However, this program also has certain drawbacks. From an aesthetic point of view, the "3 + 1 splitting" of Einstein's theory is somewhat unappealing. Also, in the work done so far, the underlying manifold structure has again been kept fixed, although, in principle, this restriction could be removed, thanks to an essentially exhaustive classification of topologies admitted by 3-manifolds equipped with asymptotically flat positive definite metrics, which has

[a)]Alfred P. Sloan Research Fellow. Supported in part by the National Science Foundation Grant PHY 80-08155.

 0022-2488/81/122885-11$01.00

now become available.[4] The more serious limitation of the program is the practical one: The constraints which arise in the Hamiltonian framework are so involved that, over the years, little progress has been made in their incorporation at the quantum level. Indeed, the state-of-the-art is such that even a kinematic framework giving the precise structure of the Hilbert space of quantum states and the algebra of observables–or substitutes thereof–is yet to be constructed.[5] It is therefore difficult even to formulate questions of physical interest. It is probably fair to say that the program is yet to "take off" in the quantum domain. Thus, overall, one has the uneasy feeling that the covariant approaches are pragmatic but not sufficiently deep for the basic problems while the canonical methods are broader in their goal but not sufficiently supple to maneuver.

The question naturally arises: can one place oneself "in between" the two schemes?

The approach that we wish to present here aims at this possibility. As in the covariant schemes, the goal is to obtain a superscattering operator, while, as in the canonical methods, the passage to quantum theory is via symplectic techniques. *However, at no stage in the analysis do we introduce a background metric, a linearization of Einstein's equation, or a* 3 + 1 *decomposition of space–time.* In particular, the underlying manifold structure is left arbitrary to a large extent. Despite this generality the resulting framework is quite rich in structure: We are able to introduce the Hilbert spaces of asymptotic quantum states, identify physically interesting operators such as energy–momentum and angular momentum, discuss the particle content of the theory, and compute spin and mass of these particles.

To achieve this, one begins with the observation that for the Maxwell field one quantizes only the radiative degrees of freedom. One wishes to do the same in the gravitational case. Fortunately, there is available, since the early sixties, a rich mathematical framework describing gravitational radiation in *exact* general relativity. The idea is to use this framework as the point of departure for quantum gravity.[6] Thus, it is only the asymptotic structure of the gravitational field at null infinity that enters the discussion directly. This fact enables one to avoid the fixation of the underlying manifold structure, the introduction of the flat background, and the 3 + 1 splitting of Einstein's theory. Finally, the BMS group at null infinity provides the machinery essential for the introduction of familiar notions in terms of which one can pose questions of physical interest. Thus, for example, gravitons now arise as asymptotic notions in the exact theory rather than as exact notions in the linear theory, and their properties such as spin and mass refer to the BMS group at null infinity rather than to the Poincaré group of a flat background space–time. More generally, one exploits the fact that, asymptotoically, Einstein's equation becomes "almost linear"; it is this simplification that enables a passage to quantum theory via symplectic techniques. Note, however, that these simplifications are not introduced by hand; the geometrical boundary conditions which must be imposed in oder that one can meaningfully talk about gravitational radiation in exact general relativity themselves imply that most nonlinearities of the exact theory are ironed out asymptotically. Finally, traces of nonlinearities do persist even at infiity, and these lead to new features in quantum theory.

The basic limitation of the approach arises from the very fact that it places itself "in between" the traditional schemes. Thus, for example, the approach is not likely to yield information on the quantum fluctuations at the Planck length except perhaps for the effect of such fluctuations on the superscattering operator. The approach is also unsuitable in the cosmological contexts. Finally, at the present stage we only have a new kinematic framework; the investigation of the $ matrix has just begun.

In this paper, we shall isolate the radiative modes of the gravitational field and investigate their properties. Section II contains certain mathematical preliminaries concerning null infinity. The radiative modes are isolated in Sec. III and properties of the "classical vacua" are discussed in Sec. IV. This discussion brings out the similiarity of the structure available in gravity with that in Yang–Mills theories. The first appendix discusses the relation between the mathematical objects introduced in the main body of the paper and the various Newman–Penrose quantities and the second extends the entire analysis to the electrovac case. The next paper will deal with the problem of quantization of these radiative modes.

II. MATHEMATICAL PRELIMINARIES

Definition: A space–time[7] $(\hat{M},\hat{g}_{ab})$ will be said to be *asymptotically* empty and flat at null inifnity[8] if there exists a space–time (M,g_{ab}) together with an imbedding of $\hat{M}$ into M (by which we shall identify $\hat{M}$ with its image in M) and a function Ω on M such that:

(i) $g_{ab} = \Omega^2 \hat{g}_{ab}$ on $\hat{M}$;

(ii) on $I := \bar{\hat{M}} - \hat{M}$, the boundary of $\hat{M}$ in M, $\Omega = 0$, $\nabla_a \Omega \neq 0$;

(iii) I is topologically $S^2 \times R$ and the restriction $\underset{\sim}{n}^a$ to I of the vector field $n^a \equiv \nabla^a \Omega$ is complete;

(iv) there exists a neighborhood N of I in M such that $\hat{g}_{ab}$ satisfies the vacuum[9] Einstein's equation, $\hat{R}_{ab} = 0$, in $N \cap \hat{M}$.

Throughout this article, we restrict ourselves to space–times which are asymptotically empty and flat in this sense. These conditions imply that the asymptotic structure of $(\hat{M},\hat{g}_{ab})$ resembles that of Minkowski space–time to a sufficient extent to enable the introduction of familiar notions such as the radiation field, peeling properties, energy–momentum 4-vectors, and conservation laws. In this section, we recall[10] how the necessary structure arises.

Conditions (i), (ii), and (iv) imply that I[11] is a null 3-surface with $\underset{\sim}{n}^a$ as normal while (iii) implies that its topological structure is $S^2 \times \mathbb{R}$. The integral curves of $\underset{\sim}{n}^a$ will be called *generators of* I. The metric g_{ab} induces, via pullback, a degenerate metric q_{ab} on I which satisfies the condition $q_{ab} \underset{\sim}{v}^b = 0$ iff $\underset{\sim}{v}^b$ is proportional to $\underset{\sim}{n}^a$. Thus, q_{ab} has signature $(0 + +)$. Next, we note that there is a certain amount of "conformal freedom": If (M,g_{ab}) is a permissible completion of $(\hat{M},\hat{g}_{ab})$ (so that the pair (M,g_{ab}) and $(\hat{M},\hat{g}_{ab})$ satisfies the conditions in the definition), then so is $(\bar{M}, \tilde{g}_{ab} = \omega^2 g_{ab})$, where ω is a nowhere vanishing smooth function on M. It is

easy to verify that one can always choose ω such that $\tilde{\nabla}_a\tilde{\nabla}_b\tilde{\Omega} \equiv \tilde{\nabla}_a\tilde{\nabla}_b\omega\Omega = 0$ on I. *We shall assume throughout that such a choice of Ω has been made.* Then, the remaining or restricted conformal freedom is $g_{ab} \to \bar{g}_{ab} = \omega^2 g_{ab}$, where $\mathcal{L}_n\omega = 0$ *on* I; i.e., $\nabla_a\nabla_b\Omega = 0$ on I if and only if $\bar{\nabla}_a\bar{\nabla}_b\bar{\Omega} = 0$ on I. In these restricted conformal frames, we have $\mathcal{L}_n q_{ab} = 0$ on I; q_{ab} is the lift to I of a positive definite metric on the 2-sphere of generators.

The derivative operator ∇_a on (M, g_{ab}) induces a derivative operator D_a on I. Since $\nabla_a g_{bc} = 0$ on M, $\nabla_a n^b = 0$ on I, and, since $\nabla_a V_b = \frac{1}{2}\mathcal{L}_V g_{ab} + \nabla_{[a}V_{b]}$ on M for any vector field V^a, we have, on I,

$$D_a q_{bc} = 0, \quad D_a n^b = 0,$$

and (1)

$$D_a V_b = \tfrac{1}{2}\mathcal{L}_V q_{ab} + D_{[a}V_{b]} \quad \text{if } V_b n^b = 0 \text{ on } I,$$

where V^c is any vector field on I such that $V^c q_{bc} = V_b$. (Note that, since $q_{bc}n^c = 0$, we can add to V^c any multiple of n^c. However, since $\mathcal{L}_n q_{ab} = 0$ and $q_{ab}n^b = 0$, $\mathcal{L}_V q_{ab}$ is unchanged under such an addition.) To compute the curvature tensor $R_{abc}{}^d$ of D, we first note that the curvature tensor $R_{abc}{}^d$ of ∇_a has the form

$$R_{abc}{}^d = \tfrac{1}{2}(g_{c[a}S_{b]}{}^d + S_{[c}\delta_{b]}{}^d) \tag{2}$$

at points *on* I, where S_{ab} is related to the Ricci tensor R_{ab} of g_{ab} via $S_{ab} = R_{ab} - \frac{1}{6}Rg_{ab}$. This comes about because the Weyl tensor $C_{abc}{}^d$ of g_{ab} vanishes *on* I. Conditions (i), (ii), and (iv) imply that $S_a{}^b$ satisfies $S_a{}^b n^a \propto n^b$ on I, whence it induces, "via pullback of the covariant index," a smooth field $S_a{}^b$ defined intrinsically on I. Finally, Eq. (2) and the fact that D is induced by ∇ imply

$$R_{abc}{}^d = \tfrac{1}{2}(q_{c[a}S_{b]}{}^d + S_{c[a}\delta_{b]}{}^d), \tag{3}$$

where $S_{ab} = S_a{}^m q_{mb}$ is the pullback to I of S_{ab}. Thus $S_a{}^b$ determines the curvature of D. The trace-free part of S_{ab} in a conformal frame in which q_{ab} is a unit 2-sphere metric is the Bondi news N_{ab} which determines the fluxes of energy–momentum and angular momentum carried away by gravitational waves. This N_{ab} satisfies

$$N_{ab} = N_{(ab)}, \quad N_{ab}n^b = 0, \quad \text{and} \quad N_{ab}q^{ab} = 0 \tag{4}$$

and has, therefore, only two linearly independent components. [Here, q^{ab} is any tensor field satisfying $q^{ab}q_{am}q_{bn} = q_{mn}$. Thus q^{ab} is determined only up to addition of terms of the form $n^{(a}V^{b)}$. This ambiguity does not affect the last of Eqs. (4) because $N_{ab}n^b = 0$.)]

Since the Weyl tensor C_{abcd} of g_{ab} vanishes *on* I, $K_{abcd} = \Omega^{-1}C_{abcd}$ admits smooth limits to I. Set $K^{ab} = K^{ambn}n_m n_n$ and $*K^{ab} = *K^{ambn}n_m n_n$. Then, since $K^{ab}n_b = *K^{ab}n_b = 0$, by restriction to I, we obtain two fields, K^{ab} and $*K^{ab}$, defined within I. Both tensor fields are symmetric and trace-free and contain physically significant information. In stationary space–times, $*K^{ab}$ vanishes identically while K^{ab} determines the Bondi mass. Thus, one might say that $*K^{ab}$ contains information only about "radiative modes" while K^{ab} contains information about "longitudinal modes" as well. Bianchi identities on (M, g_{ab}) imply that the two fields must satisfy

$$D_a *K^{ab} = 0, \quad D_a K^{ab} = 0,$$

$$D_{[a}S_{b]}{}^c = \tfrac{1}{4}\epsilon_{abm}{}^*K^{mc}. \tag{5}$$

These equations lead to the conservation law–often called the "balance equation"–relating the changes in the Bondi 4-momentum to the Bondi news N_{ab}.

This exhausts the asymptotic structure relevant to the present series of papers. To conclude this section, we note the conformal behavior of various fields. Under the transformation $g_{ab} \to \bar{g}_{ab} = \omega^2 g_{ab}$, we have

$$\begin{aligned}
&\bar{q}_{ab} = \omega^2 q_{ab}, \quad \bar{n}^a = \omega^{-1}n^a, \\
&\bar{D}_a K_b = D_a K_b - 2\omega^{-1}K_{(a}D_{b)}\omega + \omega^{-1}\omega^m K_m q_{ab}, \\
&\bar{S}_a{}^b = \omega^{-2}S_a{}^b - 2\omega^{-3}D_a\omega^b + 4\omega^{-4}\omega^b D_a\omega \\
&\qquad - \omega^{-4}\omega^m D_m\omega\delta_a{}^b, \\
&\bar{K}^{ab} = \omega^{-5}K^{ab}; \text{ and } {}^*\bar{K}^{ab} = \omega^{-5}{}^*K^{ab},
\end{aligned} \tag{6}$$

where ω^m is the restriction to $\mathscr{I}$ of $\nabla^m\omega$. (Note that, since $\mathcal{L}_n\omega = 0$ on $\mathscr{I}$, $\nabla^m\omega$ is automatically tangential to I and that ω^m satisfies $\omega^m q_{am} = D_a\omega$.)

III. ISOLATION OF THE RADIATIVE MODES

In the previous section, we fixed a space–time $(\hat{M}, \hat{g}_{ab})$ and outlined the structure available at its null infinity. In this section, we wish to consider *all* space–times which satisfy the boundary conditions of the definition. To be able to deal with this collection, we must first introduce a "kinematical arena" which will be common to all such space-times, i.e., which does not depend on the features which change from one space–time to another. In the case of nongravitational fields, the underlying space–time itself provides this arena. In the covariant approach to quantum gravity, the role is played by the "background space–time," topologically $\mathbb{R}^4$ and equipped with a flat metric n_{ab}, while in the canonical approach, the 3-manifold which ultimately turns out to be a (spacelike) Cauchy surface serves this purpose. In the present approach, we wish to impose the minimal possible restrictions on the global structures of permissible space–times. The emphasis on the quantization or radiative modes has led us to impose only boundary conditions at null infinity; the "interior" structure– including the topology–has remained pretty much unconstrained.[12] We wish to preserve theis feature. Therefore, we shall choose null infinity[13] itself as our kinematic arena. More precisely, we proceed as follows.

Fix a 3-manifold $\mathscr{I}$, topologically $\mathbb{S}^2 \times \mathbb{R}$, equipped with a collection of pairs (q_{ab}, n^a) of nowhere vanishing fields, such that: (i) $q_{ab}V^b = 0$ iff V^b is proportional to n^a; (ii) $\mathcal{L}_n q_{ab} = 0$; (iii) pairs (q_{ab}, n^b) and $(q_{ab}, \bar{n}^b)$ are in the collection iff there exists a smooth function ω on $\mathscr{I}$, such that $\bar{q}_{ab} = \omega^2 q_{ab}$ and $\bar{n}^a = \omega^{-1}n^a$; and (iv) the vector n^a is complete and the manifold $\mathscr{S}$ of its orbits is diffeomorphic to $\mathbb{S}^2$. [Note that (i), (ii), and (iii) imply that the function of ω of (iii) automatically satisfies $\mathcal{L}_n\omega = 0$.] This is the required "kinematical arena." Note that $\mathscr{I}$ is introduced here abstractly; it is not the null infinity of any specific asymptotically flat space–time.

In Minkowskian field theories, the symmetry group of the kinematical arena is the Poincaré group which then plays an important role in the entire theory. What is the corresponding group in the present case? The analysis of Schmidt, Walker, and Sommers[14] leads us to the following result:

Lemma 1.1: The subgroup of the diffeomorphism group of $\mathscr{I}$ which preserves the given collection of pairs (q_{ab}, n^a) is precisely the BMS group.

The fact that one obtains the BMS group rather than the Poincaré group will play an important role in what follows. For the present, we merely note that, given an asymptotically flat space-time $(\hat{M}, \hat{g}_{ab})$ and a completion thereof, there exists a diffeomorphism Ψ between the null boundary of $I = \hat{M} - \hat{M}$ of this space-time and $\mathscr{I}$ which preserves the preferred collection of pairs ("the universal structure") and that any two such diffeomorphisms are related by an element of the BMS group.

Next, we introduce certain fields on our kinematical arena. Denote by C the collection of torsion-free connections D on $\mathscr{I}$, satisfying

$$D_a q_{bc} = 0 \quad \text{and} \quad D_a n^b = 0 \tag{7a}$$

for any pair (q_{ab}, n^a) in our collection. Since q_{ab} is degenerate, Eq. (7a) fails to determine D uniquely. To see the available freedom, we first note a consequence of Eq. (7a):

$$D_a V_b = D_{[a} V_{b]} + \tfrac{1}{2} \mathscr{L}_V q_{ab} \quad \text{if } V_c n^c = 0, \tag{7b}$$

where, as before, V^c is any vector field on $\mathscr{I}$ such that $V^c q_{bc} = V_b$. Thus, because of Eq.(7a), the action of D or any covector field V_c satisfying $V_c n^c = 0$ is predetermined. Hence, to specify the action of D on any covector field–and therefore on arbitrary tensor fields– on $\mathscr{I}$, we need to give only $D_a l_b$ for a l_b satisfying $l_b n^b = 1$. This is the freedom available in the choice of D in any "conformal frame" (g_{ab}, n^a). Equation (7a) is clearly motivated by Eq. (1) on I. However, since $\mathscr{I}$ is not imbedded in any space–time, Eq. (7a) had just to be postulated; the derivation of Eq. (1) uses the properties of the space–time connection ∇. It will turn out, somewhat surprisingly, that one does not need to introduce additional restrictions: We shall see that the entire structure relevant to the gravitational radiation theory can be introduced starting *only* from connections D in C.

Fix a connection D in C and denote its curvature by $R_{abc}{}^d$, $D_{[a} D_{b]} K_c = \frac{1}{2} R_{abc}{}^d K_d$. Then we have

Lemma 1.2: There exists a tensor field $S_a{}^b$ on $\mathscr{I}$ satisfying (i) $S_a{}^b n^a = (S - R^0) n^a$; (ii) $S_a{}^b q_{bc} \equiv S_{ac} = S_{(ac)}$; and, (iii) $R_{abc}{}^d = \frac{1}{2}(q_{c[a} S_{b]}{}^d + S_{c[a} \delta_{b]}{}^d)$, where $S = S_a{}^a$ and R^0 is the lift to $\mathscr{I}$ of the scalar curvature of q_{ab} on the manifold $\mathscr{S}$ of orbits of n^a.

Proof: We first note the algebraic symmetries of $R_{abc}{}^d$. Since it is the curvature tensor of a torsion-free connection, we have

$$R_{abc}{}^d = R_{[ab]c}{}^d \quad \text{and} \quad R_{[abc]}{}^d = 0$$

while the second of Eqs. (7a) implies

$$n^c R_{abc}{}^d = 0.$$

Next, consider any K_c such that $K_c n^c = 0$. Equation (7b) implies that the action of any D in C on such a K_c is completely expressible in terms of Lie and exterior derivatives and is independent of the particular choice of D. It therefore follows that[15]

$$R_{abcd} := R_{abc}{}^m q_{md} = R^0{}_{abcd},$$

where $R^0{}_{abcd}$ is the lift to $\mathscr{I}$ of the Riemann tensor of q_{ab} on $\mathscr{S}$. Fix a point p of $\mathscr{I}$. The algebraic properties of $R_{abc}{}^d$ imply that the restriction to p of Riemann tensors of all connections D in C yields a five-dimensional affine space. Denote this space by $\mathscr{A}_R$. Next, consider, at p, the five-dimensional affine space $\mathscr{A}_S$ of tensors $S_a{}^b$ satisfying

$$(S_a{}^b - S\delta_a{}^b) n^a = R^0 n^a \quad \text{and} \quad S_a{}^c q_{bc} =: S_{ac} = S_{(ac)}.$$

Now, it is easy to verify that

$$S_a{}^b \to \tfrac{1}{2}(q_{c[a} S_{b]}{}^d + S_{c[a} \delta_{b]}{}^d)$$

is an affine structure preserving mapping from $\mathscr{A}_S$ into $\mathscr{A}_R$. We now wish to show that the mapping is one-to-one and hence an isomorphism. Let us suppose that $S_a{}^b$ and $S'_a{}^b$ are mapped to the same element of $\mathscr{A}_R$. Set $\Delta_a{}^b = S_a{}^b - S'_a{}^b$. This $\Delta_a{}^b$ must satisfy

$$(\Delta_a{}^b - \Delta\delta_a{}^b) n^a = 0, \quad \Delta_{ab} = \Delta_{(ab)},$$

$$q_{c[a} \Delta_{b]}{}^d + \Delta_{c[a} \delta^d{}_{b]} = 0.$$

Transvecting the last equation with n^a and using the first equation, one obtains $\Delta_{ab} = -\Delta q_{ab}$. Substituting this result back in the last equation, one has $\Delta_a{}^b = \Delta\delta_a{}^b$ which is impossible since $\Delta = \Delta_a{}^a$. Hence the mapping displayed above is an isomorphism. Thus, at any point p of $\mathscr{I}$, the Riemann tensor $R_{abc}{}^d$ of any connection D in C is expressible as

$$R_{abc}{}^d = \tfrac{1}{2}(q_{c[a} S_{b]}{}^d + S_{c[a} \delta_{b]}{}^d),$$

where $S_a{}^b$ satisfies

$$S_a{}^b n^a = (S - R^0) n^b \quad \text{and} \quad S_{ab} = S_{(ab)}. \qquad \square$$

Remarks: (1) Lemma 1.2 follows only from the algebraic properties of $R_{abc}{}^d$. Its differential properties, such as the second Bianchi identity, will give us differential equations on $S_a{}^b$. (2) The result of Lemma 1.2 is analogous to the fact that the Ricci tensor of a Riemannian connection on a three-dimensional manifold suffices to determine the entire curvature tensor. Note, however, that the connections in C are *not* necessarily Riemannian since q_{ab} is degenerate. It is because of this that we needed both of Eq. (7) to prove Lemma 1.2. (3) In Sec. II, the derivative operator D was induced on I by the space–time derivative ∇ and Eq. (3) relating $R_{abc}{}^d$ and $S_a{}^b$ followed from Eq. (2) relating the Riemann tensor $R_{abc}{}^d$ of ∇ to its Ricci tensor. Thus, the previous derivation of Eq. (3) made a crucial use of the fact that I is imbedded in the completed space–time; one used, e.g., the fact that the Weyl tensor $C_{abc}{}^d$ of g_{ab} vanishes on I. It is therefore somewhat surprising that, on $\mathscr{I}$, the analog of Eq. (3) follows directly from Eq. (7) without any reference to a space–time geometry. The basic properties of connections in C–Eqs. (7)–refer to a particular choice of "conformal frame" (q_{ab}, n^a) on $\mathscr{I}$. We need to specify the transformation properties of D under rescalings $(q_{ab}, n^a) \to (\bar{q}_{ab}, \bar{n}^a) = (\omega^2 q_{ab}, \omega^{-1} n^a)$. The specification is subject to two constraints. First, the statement of the

transformation law can refer only to that structure which is available on $\mathscr{I}$; we do *not* have access to a preferred space–time geometry. Second, given an imbedding of $\mathscr{I}$ into the completion (M, g_{ab}) of an asymptotically flat space–time $(\hat{M}, \hat{g}_{ab})$—or, more precisely, given a universal structure preserving diffeomorphism ψ between the null infinity of I of $(\hat{M}, \hat{g}_{ab})$ and $\mathscr{I}$—the transformation properties specified on $\mathscr{I}$ should reduce to Eqs. (6) on I. Let us therefore first examine Eqs. (6). Setting $\omega = 1$ on I in these equations, we have, for q_{ab}, n^a, and D,

$$\bar{q}_{ab} = q_{ab}, \quad \bar{n}^a = n^a,$$
$$\bar{D}_a K_b = D_a K_b + f q_{ab} n^m K_m, \tag{8}$$

where f is the function on I given by $f n^m = \nabla^m \omega$. (Since ω is constant on I, $\nabla^m \omega$ is necessarily proportional to n^m there.) Thus, because the derivative operator D on I contains information about space–time geometry to "second order" while q_{ab} and n^a contain information only to "first order," D can be affected by changes in the space–time conformal factor to which q_{ab} is insensitive. In terms of $\mathscr{I}$, on the other hand, we cannot distinguish between two conformal factors which agree on $\mathscr{I}$; we do not have access to fields such as $\nabla^a \omega$ which refer to space–time. We therefore introduce the equivalence relation

$$D \approx \tilde{D} \quad \text{iff} \quad (\tilde{D}_a - D_a) K_b = f q_{ab} n^c K_c \tag{9}$$

for some function of f on $\mathscr{I}$, independently of one's choice of K_a, where D and $\tilde{D}$ are connections satisfying Eqs. (7) in the conformal frame (q_{ab}, n^a). Denote by $\{D\}$ the equivalence class to which D belongs. Then, $\{D\}$ has a well-defined transformation property satisfying the two constraints: Under $(q_{ab}, n^a) \to (\bar{q}_{ab}, \bar{n}^a) = (\omega^2 q_{ab}, \omega^{-1} n^a)$ we have

$$\{\bar{D}_a\} K_b = \{D_a\} K_b + 2\omega^{-1} K_{(a} D_{b)} \omega. \tag{10}$$

where $\{D_a\} K_b$ denotes the equivalence class of tensor fields obtained by operating on K_b various elements of $\{D\}$. It turns out that these equivalence classes, $\{D\}$, are the basic dynamical variables representing the radiative modes of the (exact, nonlinear) gravitational field. Transformations $D \to \tilde{D}$ where D and $\tilde{D}$ are related by Eq. (9) will therefore be regarded as gauge transformations. Under such a change, we have

$$S_a{}^b \to \tilde{S}_a{}^b = S_a{}^b - 2(D_a f) n^b. \tag{11}$$

Fix a conformal frame (q_{ab}, n^a) and consider connections D satisfying Eqs. (7). Denote by Γ the space of equivalence classes $\{D\}$ subject to the relations in Eq. (9). [Under a conformal rescaling, $(q_{ab}, n^a) \to (\bar{q}_{ab}, \bar{n}^a)$, $\{D\}$ is mapped to $\{\bar{D}\}$ according to Eq. (10). Hence, if we know Γ in one conformal frame, we know it in any other.] *This Γ is the space of radiative modes.* To show this, we proceed in two steps. First, we show that $\{D\}$ has precisely two degrees of freedom.

Lemma 1.3: The difference between any two elements $\{D\}$ and $\{D'\}$ of Γ can be completely characterized by a symmetric tensor field γ_{ab} on $\mathscr{I}$ satisfying $\gamma_{ab} n^b = 0$ and $\gamma_{ab} q^{ab} = 0$, where q^{ab} is any tensor field satisfying

$$q^{ab} q_{am} q_{bn} = q_{mn}.$$

Proof: Since D and D' are torsion-free connections, we have $(D'_a - D_a) K_b = C_{ab}{}^c K_c$ for some tensor field $C_{ab}{}^c$ satisfying $C^c_{ab} = C^c_{(ab)}$. Since $D_a q_{bc} = 0 = D'_a q_{bc}$, we have $C_{ab}{}^c = \Sigma_{ab} n^c$ for some symmetric tensor field C_{ab}. Next, since $D_a n^b = 0 = D'_a n^b$, we have $\Sigma_{ab} n^b = 0$. Finally, Eq. (9) implies that $D \approx D'$, i.e., $\{D\} = \{D'\}$, if and only if Σ_{ab} is proportional to q_{ab}. Hence $\{D\} - \{D'\}$ is completely characterized by $\gamma_{ab} = \Sigma_{ab} - \frac{1}{2}(\Sigma_{mn} q^{mn}) q_{ab}$, which, by construction, satisfies

$$\gamma_{ab} n^b = 0 \text{ and } \gamma_{ab} q^{ab} = 0. \qquad \square$$

The algebraic properties of γ_{ab} imply that it has precisely two independent components. These represent the radiative degrees of freedom of the gravitational field.[16]

The second and more important reason for regarding $\{D\}$ as the fundamental dynamical variable representing radiative modes is that all the information about radiative aspects of gravity can be extracted out of $\{D\}$. To show this, we begin by recalling the following result.

Lemma 1.4: On $\mathscr{I}$, there exists a unique symmetric tensor field ρ_{ab} satisfying $\rho_{ab} n^b = 0$, $\rho_{ab} q^{ab} = R^0$ and $D_{[a} \rho_{b]c} = 0$, where R^0 is the pullback to $\mathscr{I}$ of the scalar curvature on $(\mathscr{S}, q_{ab})$ and D is any connection in C.

Proof: See Ref. 10, p. 34.

Remark: Fix a conformal frame (q_{ab}, n^a) on $\mathscr{I}$ such that q_{ab} is a 2-sphere metric on $\mathscr{S}$. [Such a (q_{ab}, n^a) will be called a Bondi conformal frame.] ρ_{ab} is then given by $\rho_{ab} = \frac{1}{2} R^0 q_{ab}$. In any other frame $(\bar{q}_{ab}, \bar{n}^b) = (\omega^2 q_{ab}, \omega^{-1} n^a)$ we have

$$\bar{\rho}_{ab} = \rho_{ab} - 2\omega^{-1} D_a D_b \omega + 4\omega^{-2} D_a \omega D_b \omega - \omega^{-2} q_{ab} (q^{mn} D_m \omega D_n \omega).$$

Using S_{ab} and ρ_{ab} we can now define the Bondi news N_{ab} and the radiation field ${}^*K^{ab}$:

$$N_{ab} := S_{ab} - \rho_{ab}, \quad {}^*K^{ab} := 2\epsilon^{amn} D_m S_n{}^b. \tag{12}$$

We shall first show that N_{ab} and ${}^*K_{ab}$ are gauge-invariant, i.e., that they depend only on equivalence classes $\{D\}$ in Γ rather than on individual connections D in C.

Lemma 1.5: If $D \approx \tilde{D}$ in the sense of Eq. (9), then $\tilde{N}_{ab} = N_{ab}$ and ${}^*\tilde{K}^{ab} = {}^*K^{ab}$.

Proof: Let $D \approx \tilde{D}$. Then there exists a function f on $\mathscr{I}$ such that, for all K_a, $(\tilde{D}_a - D_a) K_b = f q_{ab} n^c K_c$. From Eq. (11), we therefore have $\tilde{S}_a{}^b = S_a{}^b - 2 D_a f n^b$ and hence $\tilde{S}_{ab} = S_{ab}$. Since ρ_{ab} is a fixed tensor field on $\mathscr{I}$, independent of the choice of connection, we have $\tilde{N}_{ab} = N_{ab}$. Next, using the definition of ${}^*K^{ab}$, we have

$${}^*\tilde{K}^{ab} = 2\epsilon^{amn} \tilde{D}_m \tilde{S}_n{}^b = 2\epsilon^{amn} D_m S_n{}^b - 4\epsilon^{amn} (D_m D_n f) n^b = {}^*K^{ab}. \qquad \square$$

Next, we show that N_{ab} and ${}^*K^{ab}$, defined here using only equivalence classes $\{D\}$ have the same properties as the fields $\underset{\_}{N}_{ab}$ and ${}^*\underset{\_}{K}{}^{ab}$ induced on I by the various space-time fields.

Lemma 1.6: N_{ab} and ${}^*K^{ab}$ satisfy $N_{ab} = N_{(ab)}$, $N_{ab} n^b = 0$, $N_{ab} q^{ab} = 0$, ${}^*K^{ab} = {}^*K^{(ab)}$, ${}^*K^{ab} q_{ab} = 0$, and $D_a {}^*K^{ab} = 0$.

Proof: By Lemma 1.2, S_{ab} is symmetric and satisfied $S_{ab} n^b = 0$. By Lemma 1.4, ρ_{ab} has the same properties. Hence $N_{ab} = N_{(ab)}$ and $N_{ab} n^b = 0$. Using again the result $S_a{}^b n^a = (S - R^0) n^b$ of Lemma 1.2 and the fact that $S_{ac} = S_a{}^b q_{bc}$, it is easy to verify that $S_{ab} q^{ab} = R^0$. Since $\rho_{ab} q^{ab} = R^0$, we have $N_{ab} q^{ab} = 0$. Next, consider ${}^*K^{ab}$. The Bianchi identity $D_{[m} R_{ab]c}{}^d = 0$ together with the expression

of $R_{abc}{}^{d}$ in terms of $S_a{}^b$ and the definition of $*K^{ab}$ implies that $*K^{[ab]}q_{ca} = 0$. Since $q_{ca}V^c = 0$ only if V_c is proportional to n^c, we have $*K^{[ab]} = 0$. The trace-free property of $*K^{ab}$ follows from its definition and the fact that S_{ab} is symmetric. Finally, by taking the divergence of $*K^{ab}$, we obtain

$$\begin{aligned} D_a *K^{ab} &= 2\epsilon^{amn} D_a D_m S_n{}^b = \epsilon^{amn}(R_{amn}{}^p S_p{}^b - R_{amp}{}^b S_n{}^p) \\ &= -\tfrac{1}{2}\epsilon^{amn}(q_{pa}S_m{}^b + S_{pa}\delta_m{}^b)S_n{}^p \\ &= -\tfrac{1}{4}(\epsilon^{amn}S_{na}S_m{}^b - \epsilon^{abn}S_{pa}S_n{}^p) = 0. \end{aligned}$$ □

Finally, let us examine the effect of conformal rescalings $(q_{ab}, n^a) \to (\bar{q}_{ab}, \bar{n}^a)$ on N_{ab} and $*K^{ab}$. Since these fields depend on equivalence classes $\{D\}$ rather than on individual connections D, one expects that they will have well-defined transformation properties. This is indeed the case. A straightforward calculation yields

$$\begin{aligned} \{\bar{S}_a{}^b\} = \omega^{-2}\{S_a{}^b\} &= 2\omega^{-3}D_a\omega^b \\ &+ 4\omega^{-4}\omega^b D_a\omega - \omega^{-4}\omega^m D_m\omega\delta_a{}^b \end{aligned}$$

where $\{S_a{}^b\}$ is the equivalence class of tensors obtained from $\{D\}$ and ω^a is *any* covector field satisfying $\omega^b q_{ab} = D_a\omega$. Hence, one has

$$\begin{aligned} \bar{S}_{ab} &= S_{ab} - 2\omega^{-1}D_aD_b\omega + 4\omega^{-2}D_a\omega D_b\omega \\ &\quad - \omega^{-2}q_{ab}(q^{mn}D_m\omega D_n\omega), \\ \bar{N}_{ab} &= N_{ab}, \quad *\bar{K}^{ab} = \omega^{-5} *K^{ab} \end{aligned} \tag{13}$$

Thus, although N_{ab} and $*K^{ab}$ have been introduced on $\mathscr{I}$ using only the equivalent class $\{D\}$, they automatically possess all the properties of the fields $\underset{\sim}{N}_{ab}$ and $*\underset{\sim}{K}^{ab}$ induced on the null infinity I of asymptotically flat space-times. That is, the discussion of this section demonstrates that the use of fields and equations from the interior of space-time, made in Ref. 10 to establish these properties, is for convenience only; the properties in fact stem directly from the structure available on the equivalence class $\{D\}$ defined intrinsically on $\mathscr{I}$. Thus, we have

Theorem 1: Let $(\hat{M}, \hat{g}_{ab})$ be an asymptotically empty and flat space–time and (M, g_{ab}) any completion thereof. Fix a universal structure preserving diffeomorphism Ψ from the null infinity I of $(\hat{M}, \hat{g}_{ab})$ onto $\mathscr{I}$ and let D denote the image under Ψ of the connection $\underset{\sim}{D}$ on I. Then, the fields N_{ab} and $*K^{ab}$ defined directly on $\mathscr{I}$ by $\{D\}$ are the images of the fields $\underset{\sim}{N}_{ab}$ and $*\underset{\sim}{K}^{ab}$ induced on I by the curvature tensor of g_{ab}.

Note that fields such as $\underset{\sim}{K}^{ab}$ cannot be introduced in terms of $\{D\}$ alone; $\{D\}$ does not contain information about longitudinal modes. (This aspect will become transparent in the next section and Appendix A.) Hence the space Γ of all permissible $\{D\}$ may indeed be regarded as the phase space[17] of radiative modes in exact general relativity. Further support in favor of this interpretation comes from the interaction of the BMS group with Γ. One can show that Γ admits a natural symplectic Ω and the BMS action on $\mathscr{I}$ induces canonical transformations on (Γ, Ω); the symmetry group of the kinematical arena also preserves the phase space structure of the dynamical variables. The corresponding generating functions can be computed. These yield the expressions of fluxes of supermomenta and angular momenta through $\mathscr{I}$.[18]

IV. CLASSICAL VACUA

Following the terminology commonly used in gauge theories, we shall call an element $\{\mathring{D}\}$ of Γ a *classical vacuum* if its curvature tensor is trivial,[19] i.e., if the corresponding fields $\mathring{N}_{ab}$ and $*\mathring{K}^{ab}$ vanish identically. In this section, we shall investigate the structure available on the collection Γ_V of these vacua and compare the situation with that in the Yang-Mills theory. The relevance of this structure to quantum theory will become clear in the next paper.

Lemma 2.1: Fix a conformal frame (q_{ab}, n^b) on $\mathscr{I}$ and an element D of C. Let t_a be the lift to $\mathscr{I}$ of a covector field $\mathbf{t}_a$ on the space $\mathscr{S}$ of generators. Then $D_a t_b$ is the lift to $\mathscr{I}$ of $\mathbf{D}_a\mathbf{t}_b$, where $\mathbf{D}$ is the connection on $\mathscr{S}$ compatible with $\mathbf{q}_{ab}$, the projection to $\mathscr{S}$ of q_{ab}.

Proof: Since t_a is the lift to $\mathscr{I}$ of a covector field on $\mathscr{S}$, we have $\mathscr{L}_n t_a = 0$ and $n^a t_a = 0$. Hence, it follows that

$$\begin{aligned} \mathscr{L}_n D_a t_b &= (\mathscr{L}_n D_a - D_a\mathscr{L}_n)t_b \\ &= n^m(D_mD_a - D_aD_m)t_b = n^m R_{mab}{}^c t_c \\ &= \tfrac{1}{2}n^m(q_{b[m}S^c{}_{a]} + S_{b[n}\delta_a{}^c{}_{]})t_c = 0; \end{aligned}$$

$n^a D_a t_b = 0$ and $n^b D_a t_b = 0$. Hence $D_a t_b$ is also a lift to $\mathscr{I}$ of a covariant tensor field $\mathbf{t}_{ab}$ on $\mathscr{I}$. Thus, the derivative operator D on $\mathscr{I}$ provides us a mapping from covector fields $\mathbf{t}_a$ to tensor fields $\mathbf{t}_{ab}$ on $\mathscr{S}$. This mapping is linear ($\mathbf{t}_b \to \mathbf{t}_{ab}$ and $\mathbf{S}_b \to \mathbf{S}_{ab} \Rightarrow \mathbf{t}_b + \mathbf{S}_b \to \mathbf{t}_{ab} + \mathbf{S}_{ab}$) and satisfies the Liebnitz rule ($\mathbf{t}_b \to \mathbf{t}_{ab} \Rightarrow \mathbf{f}\mathbf{t}_b \to \mathbf{f}\mathbf{t}_{ab} + \mathbf{t}_b\mathbf{D}_a\mathbf{f}$ for all functions $\mathbf{f}$ on $\mathscr{S}$). Hence, there exists a torsion-free connection $\mathbf{D}_a$ on $\mathscr{S}$ such that $\mathbf{t}_{ab} = \mathbf{D}_a\mathbf{t}_b$. Finally, since $D_a q_{bc} = 0$ on $\mathscr{I}$, it follows that $\mathbf{D}_a\mathbf{q}_{bc} = 0$. Thus $D_a t_b$ is the lift to $\mathscr{I}$ of $\mathbf{D}_a\mathbf{t}_b$, where $\mathbf{D}$ is the derivative operator on $(\mathscr{S}, q_{ab})$. □

Lemma 2.2: Let (q_{ab}, n^a) be a Bondi conformal frame, i.e., let q_{ab} be a 2-sphere metric on $\mathscr{S}$. Let Σ_{ab} be a symmetric tensor field on $\mathscr{I}$ satisfying $n^a\Sigma_{ab} = 0$ and $D_{[a}\Sigma_{b]c} = 0$. Then there exists a function f on $\mathscr{I}$ such that $\mathscr{L}_n f = 0$ and $\Sigma_{ab} = D_aD_bf + R^0 f q_{ab}$ where the constant R^0 is the pullback to $\mathscr{I}$ of the scalar curvature on $(\mathscr{S}, \mathbf{q}_{ab})$.

Proof: We have $\mathscr{L}_n\Sigma_{bc} = n^aD_a\Sigma_{bc} = 2n^aD_{[a}\Sigma_{b]c} = 0$. Since $\Sigma_{ab}n^b$ also vanishes, Σ_{ab} is the lift to $\mathscr{I}$ of a tensor field Σ_{ab} on $\mathscr{S}$. Hence, by Lemma 2.1, $D_a\Sigma_{bc}$ is the lift of $\mathbf{D}_a\Sigma_{bc}$ whence $\mathbf{D}_{[a}\Sigma_{b]c} = 0$. Thus, on the metric 2-sphere $(\mathscr{S}, \mathbf{q}_{ab})$ we have a symmetric tensor field Σ_{ab} satisfying $\mathbf{D}_{[a}\Sigma_{b]c} = 0$, where $\mathbf{D}$ is the derivative operator compatible with $\mathbf{q}_{ab}$. Hence, there exists a function $\mathbf{f}$ on $\mathscr{S}$ such that $\Sigma_{ab} = \mathbf{D}_a\mathbf{D}_b\mathbf{f} + R^0\mathbf{f}\mathbf{q}_{ab}$. Let f be the pullback to $\mathscr{I}$ of $\mathbf{f}$. Then, by Lemma 2.1, D_aD_bf is the pullback of $\mathbf{D}_a\mathbf{D}_b f$ whence $\Sigma_{ab} = D_aD_bf + R^0 f q_{ab}$. □

Using these two lemmas, we can now prove the main result concerning the structure of the space Γ_V of classical vacua.

Theorem 2: Γ_V is an affince subspace of Γ on which the quotient group ST/T acts simply and transitively, where ST is the group of BMS supertranslations and T of BMS translations.

Proof: Fix a Bondi conformal frame (q_{ab}, n^a) on $\mathscr{I}$ and consider an element $\{\mathring{D}\}$ of Γ_V. Since $\mathring{N}_{ab}$ vanishes, $\mathring{S}_{ab} = \rho_{ab} \equiv \tfrac{1}{2}R^0 q_{ab}$ for any connection $\mathring{D}$ in $\{\mathring{D}\}$, where R^0 is the pullback to $\mathscr{I}$ of the scalar curvature of $(\mathscr{S}, \mathbf{q}_{ab})$. Hence $\mathring{S}_a{}^b = \tfrac{1}{2}R^0\delta_a{}^b + f_a n^b$ for some covector field f_a. Since

$^*K^{ab} = 0$, $D_{[a}f_{b]} = 0$ whence $f_b = D_b f$ for some function f. Thus, $\mathring{S}_a{}^b = \frac{1}{2}R^0\delta_a{}^b + D_a f n^b$. Therefore, one can always find and element $\mathring{D}$ of $\{\mathring{D}\}$ for which $\mathring{S}_a{}^b = \frac{1}{2}R^0\delta_a{}^b$ [See Eq. (11)]. Next, consider two elements $\{\mathring{D}\}$ and $\{\mathring{D}'\}$ of Γ_V and let $\mathring{D}$ and $\mathring{D}'$ be such that $\mathring{S}_a{}^b = \mathring{S}'_a{}^b = \frac{1}{2}R^0\delta_a{}^b$. Let $\mathring{\Sigma}_{ab}$ characterize the difference between $\mathring{D}$ and $\mathring{D}'$, i.e., let $(\mathring{D}'_a - \mathring{D}_a)K_b = \mathring{\Sigma}_{ab}n^cK_c$. $\mathring{\Sigma}_{ab}$ is symmetric[20] and satisfies $\mathring{\Sigma}_{ab}n^a = 0$. Next, since $\mathring{S}_a{}^b = \mathring{S}'_a{}^b$, $\mathring{D}$ and $\mathring{D}'$ have the same curvature. Hence, we have

$$
\begin{aligned}
0 &= \mathring{D}'_{[a}\mathring{D}'_{b]} - \mathring{D}_{[a}\mathring{D}_{b]})K_c \\
&= \mathring{D}_{[a}\mathring{D}'_{b]}K_c + \mathring{\Sigma}_{c[a}n^p\mathring{D}'_{b]}K_p - \mathring{D}_{[a}\mathring{D}_{b]}K_c \\
&= \mathring{D}_{[a}\mathring{D}_{b]}K_c + \mathring{D}_{[a}(\mathring{\Sigma}_{b]c}n^pK_p) + \mathring{\Sigma}_{c[a}\mathring{D}'_{b]}n^pK_p \\
&\quad - \mathring{D}_{[a}\mathring{D}_{b]}K_c = n^pK_p\mathring{D}_{[a}\mathring{\Sigma}_{b]c} \quad \text{for any } K_c.
\end{aligned}
$$

Hence, we have $\mathring{D}_{[a}\Sigma_{b]c} = 0$. Thus, on $(\mathscr{I}, q_{ab}, n^a, \mathring{D})$, $\mathring{\Sigma}_{ab}$ fulfills the conditions of Lemma 2.2. Therefore, there must exist a function f on $\mathscr{I}$ satisfying $\mathscr{L}_n f = 0$ and $\mathring{\Sigma}_{ab} = \mathring{D}_a\mathring{D}_b f + R^0 f q_{ab}$. Conversely, it is easy to check (by running the argument backwards) that, given a connection $\mathring{D}$ with trivial curvature, $\mathring{D}'$, defined by $\mathring{D}'_aK_b = \mathring{D}_aK_b + (\mathring{D}_a\mathring{D}_b f + fR^0q_{ab})n^cK_c$ is again an element of C with trivial curvature. Thus, the subspace of C consisting of connections with trivial curvatures is an affine space. Hence it follows that the space Γ_V of classical vacua is an affine subspace of Γ. The tangent space within Γ_V of any $\{\mathring{D}\}$ is spanned by tensor fields $\mathring{\gamma}_{ab}$ on $\mathscr{I}$ of the form $\mathring{\gamma}_{ab} \hat{=} \mathring{\Sigma}_{ab} \hat{=} \mathring{D}_a\mathring{D}_b f$, where f satisfies $\mathscr{L}_n f = 0$ and where $\hat{=}$ stands for "equal to the trace-free part of."

Next, consider the action of a BMS supertranslation vector field, fn^a, on Γ_V. For any connection $\mathring{D}$ with trivial curvature and any K_b, we have $(\mathscr{L}_{\alpha n}\mathring{D}_a - \mathring{D}_a\mathscr{L}_{\alpha n})K_b$
$= (\alpha n^m R^0{}_{mab}{}^p + \mathring{D}_a\mathring{D}_b\alpha n^p)K_p$
$= (\mathring{D}_a\mathring{D}_b\alpha - \frac{1}{4}(\mathring{S} - R^0/2)n^pK_p$. Consider the one-parameter family $S(\lambda)$ of BMS supertranslations generated by αn^a. Denote by $S(\lambda)\circ\{\mathring{D}\}$ the images of a classical vacuum $\{\mathring{D}\}$. Then, $\gamma_{ab}(\lambda)$ characterizing $\overrightarrow{S(\lambda)}\circ\{\mathring{D}\} - \{\mathring{D}\}$ is given by $\gamma_{ab}(\lambda) \hat{=} \lambda\mathring{D}_a\mathring{D}_b\alpha$. Since α satisfies $\mathscr{L}_n\alpha = 0$, it follows that the images $\overrightarrow{S(\lambda)}\circ\{\mathring{D}\}$ are again classical vacua. Thus, the action of BMS supertranslations leaves Γ_V invariant. Consider a supertranslation αn^a whose action leaves each element $\{\mathring{D}\}$ of Γ_V individually invariant. This is possible if and only if $\gamma_{ab}(\lambda) = 0$, i.e., if and only if $\mathring{D}_a\mathring{D}_b\alpha$ is proportional to q_{ab}. Since q_{ab} is a 2-sphere metric, this condition can hold if and only if α is a BMS translation. Thus, the supertranslations whose action on Γ_V leaves each point of Γ_V invariant are precisely the translations. Hence the group ST/T acts on Γ_V and the action is simple; the only element of ST/T which maps each element of Γ_V to itself is the identity.

Finally, we show that the action is transitive. Fix any two classical vacua $\{\mathring{D}\}$ and $\{\mathring{D}'\}$. Then, there exists a function f on $\mathscr{I}$ such that $\mathscr{L}_n f = 0$ and $\gamma_{ab} \hat{=} \mathring{D}_a\mathring{D}_b f$, where γ_{ab} characterizes $\{\mathring{D}'\} - \{\mathring{D}\}$. Hence the supertranslation generated by fn^a for the parameter value $\lambda = 1$ maps $\{\mathring{D}\}$ to $\{\mathring{D}'\}$. □

Intuitively, Theorem 2 may be interpreted as saying that there are "as many classical vacua $\{\mathring{D}\}$ as there are elements of ST/T." Note, however, that there is no *natural* isomorphism between Γ_V and ST/T. Indeed, Γ_V is an affine space while ST/T has a natural vector space structure. This situation is analogous to that w.r.t the Poincaré subgroups of the BMS group: there are "as many Poincaré subgroups of the BMS group as there are elements of ST/T", although there is no natural correspondence between the two. One might therefore suspect that a natural isomorphism may exist between Γ_V and the set S_p of Poincaré subgroups. This is indeed the case: The addition of an arbitrarily chosen but fixed classical vacuum to the structure that must be preserved by the asymptotic symmetry group causes a canonical reduction of the BMS group to the Poincaré. Thus, we have the following result.

Theorem 3: There is a natural isomorphism between Γ_V and S_p.

Proof: We shall explicitly exhibit the required isomorphism. Fix a conformal frame (q_{ab}, n^a) and a classical vacuum $\{\mathring{D}\}$, where $\mathring{D}$ satisfies Eq. (7a) w.r.t. (q_{ab}, n^a). We shall first show that the subgroup G of the BMS group which sends $(q_{ab}, n^a, \{\mathring{D}\})$ to $(\bar{q}_{ab}, \bar{n}^a, \{\bar{\mathring{D}}\})$ is a Poincaré group. (Here $\bar{q}_{ab} = \omega^2 q_{ab}$, $\bar{n}^a = \omega^{-1}n^a$, and $\{\bar{\mathring{D}}_a\}K_b$
$= \{\mathring{D}_a\}K_b - 2\omega^{-1}K_{(a}D_{b)}\omega$ for *some* ω.)

For convenience, let us work with the BMS Lie algebra rather than the BMS group. Fix a BMS vector field ξ^a (so that $\mathscr{L}_\xi q_{ab} = 2kq_{ab}$ and $\mathscr{L}_\xi n^a = -\kappa n^a$ for some function k on $\mathscr{I}$). For simplicity, let us suppose that there exists a Bondi frame (q'_{ab}, n'^a) such that $\mathscr{L}_\xi q'_{ab} = 0$ and $\mathscr{L}_\xi n'^a = 0$. Fix a $\mathring{D}'$ in the equivalence class $\{\mathring{D}'\}$. Now, a straightforward calculation yields $(\mathscr{L}_\xi\mathring{D}'_a - \mathring{D}'_a\mathscr{L}_\xi)K_b = \Sigma_{ab}n^cK_c$, where $\Sigma_{ab} = R'^0\xi'_b l_a - R'^0(\xi^c l_c)q'_{ab} - l_c\mathring{D}'_a\mathring{D}'_b\xi^c$, where $\xi'_b = \xi^a q'_{ab}$ and where l_c is any covector field on $\mathscr{I}$ such that $l_c n^c = 1$. It is easy to verify that $\Sigma_{ab}n^b = 0$ and $\mathring{D}'_{[a}\Sigma_{b]c} = 0$. Hence, by Lemma 2.2, there exists a function f on $\mathscr{I}$ such that $\mathscr{L}_n f = 0$ and $\Sigma_{ab} = \mathring{D}'_a\mathring{D}'_b f + R'^0 f q'_{ab}$. Set $\tilde{\xi}^a = \xi^a - fn^a$. Since $\tilde{\xi}^a - \xi^a$ is a BMS supertranslation, $\tilde{\xi}^a$ is also a BMS vector field (satisfying $\mathscr{L}_{\tilde{\xi}}q_{ab} = 2kq_{ab}$, $\mathscr{L}_{\tilde{\xi}}n^a = -kn^a$). Furthermore, as shown in the proof of Theorem 2, $(\mathscr{L}_{fn}\mathring{D}'_a - \mathring{D}'_a\mathscr{L}_{fn})K_b$
$= (\mathring{D}'_a\mathring{D}'_b f - \frac{1}{4}(\mathring{S}' - R^{0\prime}/2)q'_{ab})n^cK_c$. Hence, it follows that $\mathscr{L}_{\tilde{\xi}}\{D'_a\}K_b = \{\mathring{D}'_a\}\mathscr{L}_{\tilde{\xi}}K_b$. Transforming this result back to the conformal frame (q_{ab}, n^a), we have $\mathscr{L}_{\tilde{\xi}}\{D_a\}K_b = \{D_a\}\mathscr{L}_{\tilde{\xi}}K_b - 2K_{(a}D_{b)}k$. Thus, the one-parameter family of BMS transformations generated by $\tilde{\xi}$ belongs to the group G. Since $\mathscr{L}_{\alpha n}\{D'_a\}K_b = \{D'_a\}\mathscr{L}_{\alpha n}K_b$ if and only if αn^a is a BMS translation vector field, $\tilde{\xi}^a + \alpha n^a$ will also have this property if and only if αn^a is a translation. Thus, given *any* BMS vector field ξ^a, there exists a supertranslation fn^a such that $\tilde{\xi}^a = \xi^a - fn^a$ belongs to the Lie algebra of G and fn^a is uniquely determined up to an addition of a BMS translation. Hence G is a Poincaré subgroup of the BMS group.

Thus, we have exhibited a mapping from Γ_V into S_p. We now show that the mapping is one-to-one and onto. Fix a Bondi conformal frame (q_{ab}, n^a) and consider two distinct classical vacua $\{\mathring{D}\}$ and $\{\bar{\mathring{D}}\}$. Then, there exists a function f on $\mathscr{I}$ such that $\mathscr{L}_n f = 0$ and $\gamma_{ab} \hat{=} \mathring{D}_a\mathring{D}_b f$, where γ_{ab} characterizes $\{\bar{\mathring{D}}\} - \{\mathring{D}\}$. Denote by G and $\bar{G}$ the Poincaré

groups selected by $\{\mathring{D}\}$ and $\{\tilde{\mathring{D}}\}$. By definition, a BMS vector field ξ^a will belong to the Lie algebra of G if and only if it has the following property: If $\mathscr{L}_\xi q_{ab} = 2kq_{ab}$, then $\mathscr{L}_\xi\{\mathring{D}_a\}K_b = \{\mathring{D}_a\}\mathscr{L}_\xi K_b - 2K_{(a}\mathring{D}_{b)}k$. It is easy to verify that ξ^a satisfies this property if and only if $\tilde{\xi}^a = \xi^a - fn^a$ satisfies the corresponding property w.r.t. $\{\tilde{\mathring{D}}_a\}$. That is, $\tilde{G}$ is the image of G under the inner automorphism generated on the BMS group by the supertranslation fn^a. Hence $G = \tilde{G}$ if and only if f is a translation, i.e., $\gamma_{ab} = 0$, whence $\{\mathring{D}\} = \{\tilde{\mathring{D}}\}$. Thus, the mapping is one-to-one. Finally, since any Poincaré subgroup of the BMS group is the image of a fixed Poincaré subgroup under the inner automorphism generated by *some* supertranslation, the mapping is also onto. □

Remarks: (1) The explicit form of the isomorphism between Γ_V and S_p shows that it commutes with the action of ST/T which can be defined independently on the two sets.

(2) Fix a *stationary* space–time which is asymptotically empty and flat at null infinity. Then, on null infinity, I, of this space-time, we have $N_{ab} = 0$, $^*K^{ab} = 0$, and $K^{ab} = fn^a n^b$ for some function f satisfying $\mathscr{L}_n f = 0$. Fix an universal structure preserving isomorphism ψ from I to $\mathscr{I}$. Then, by Theorem 1, the image under ψ of the connection on I has trivial curvature and thus defines a vacuum $\{\mathring{D}\}$ in Γ. Note, however, that the precise vacuum $\{\mathring{D}\}$ on $\mathscr{I}$ depends on the choice of ψ: Theorems 2 and 3 imply that one can obtain any desired vacuum by suitable choosing ψ. Thus, one cannot distinguish between two stationary space-times in terms of the imprint they leave in Γ. This is to be expected since Γ is the space of radiative modes which are absent in the stationary context.

(3) This discussion also shows that the vacuum degeneracy is redundant. That is, unlike in the Yang-Mills theory, here all vacua are "trivial"; there does not exist a "topological quantum number" to distinguish between them. Rather, the situation is similar to (1 + 1)-dimensional models such as the sine-Gordon field, where the vacuum degeneracy is again trivial. In the sine-Gordon case, classical vacua are $\phi(x,t) = \pm n\pi$ and it is the field configuration $\phi(x,t)$ (satisfying $\mathrm{Lim}_{x\to\infty}\,\phi(x) = n\pi$, $\mathrm{Lim}_{x\to\infty}\,\phi(x,t) = m\pi$, $m \neq n$) connecting two distinct vacua–rather than the individual vacua themselves–that lead to interesting structure in the quantum theory. Theorems 2 and 3 show that the enlargement of the Poincaré group to the BMS occurs in classical general relativity precisely because of the presence of physically interesting configurations $\{D\}$ which tend to distinct classical vacua $\{\mathring{D}_+\}$ and $\{\mathring{D}_-\}$ as the affine parameter u along n^a tends to $\pm\infty$. We shall see in the next paper that the presence of these configurations intertwines the supertranslation ambiguities in the classical radiation theory with the infrared problems in the quantum theory.

To conclude this discussion, let us compare and contrast the structure available in the gravitational case with that of gauge theories.[21] The broad analogy between the two is quite striking. In both cases, the basic dynamical variables are connections, and physical observables such as energy-momentum and angular momentum are constructed from the curvature tensors of these connections. Next, in both cases, there is vacuum degeneracy, i.e., there exist several distinct connections with trivial curvature. Indeed, if we restrict ourselves to "trivial" vacua in the Yang-Mills case, the qualitative analogy extends to detailed mathematical properties. To see this, let us briefly recall[22] the situation in the Yang–Mills theory. Here, the action of any connection is completely specified by its action on a basis $e^\alpha{}_{\mathcal{A}}$, where α is an internal index ("abstract" in the sense of Penrose[23]) and α takes values between 1 and $N \equiv$number of internal degrees of freedom. Given a connection $\mathring{D}$ with zero curvature, $\mathring{D}_{[a}\mathring{D}_{b]}K^\alpha \equiv F_{ab}{}^\alpha{}_\beta K^\beta = 0$, there exists a basis field $e^\alpha{}_{\mathcal{A}}$ in space-time such that $\mathring{D}_a e^\alpha{}_{\mathcal{A}} = 0$, and, if $e^\alpha{}_{\mathcal{A}}$ and $e'{}_{\alpha\mathcal{A}}$ are two bases which are constant in this sense w.r.t. $\mathring{D}$, then they differ by a *global* gauge transformation. Thus, there is a one-to-one correspondence between connections $\mathring{D}$ with vanishing curvature and equivalence classes of basis fields where two are regarded as equivalent if they differ by a global gauge transformation. Consequently, it is the quotient G_L/G of the local gauge group G_L by the global gauge group G that acts simply and transitively on the collection of vacua D. In performing calculations, it is often more convenient to deal with tensor fields than derivative operators. One therefore fixes a classical vacuum $\mathring{D}$ as the "origin" in the affine space of connections and labels any other connection D by the field $A_a{}^\alpha{}_\beta$ given by $(D_a - \mathring{D}_a)K^\alpha = A_a{}^\alpha{}_\beta K^\beta$. However, because of the vacuum degeneracy, there is some freedom in the choice of $A_a{}^\alpha{}_\beta$: since any two vacua $\mathring{D}$ and $\mathring{D}'$ are related by $(\mathring{D}'_a - \mathring{D}_a)K^\alpha = (\Lambda^{-1})^\alpha{}_\gamma \mathring{D}_a \Lambda^\gamma{}_\beta$, where $\Lambda^\alpha{}_\beta$ relates the bases $e^\alpha{}_\alpha$ and $e'^\alpha{}_\alpha$ selected by $\mathring{D}$ and $\mathring{D}'$, respectively, the change of origin $\mathring{D}\to\mathring{D}'$ changes the label $A_a{}^\alpha{}_\beta$ by $A_a{}^\alpha{}_\beta \to A'_a{}^\alpha{}_\beta = A_a{}^\alpha{}_\beta + (\Lambda^{-1})^\alpha{}_\gamma D_a \Lambda^\gamma{}_\beta$. Finally, one often wishes to deal with components $A_a{}^\alpha{}_{\mathcal{B}} = A_a{}^\alpha{}_\beta e^\beta{}_{\mathcal{B}}$ of $A_a{}^\alpha{}_\beta$, where $e^\alpha{}_\alpha$ is the basis selected by the "origin" $\mathring{D}$. Under change of origin, the basis also changes, whence we have the familiar property $A_a{}^\alpha{}_\beta \to A'_a{}^\alpha{}_\beta = \Lambda^\alpha{}_\gamma A_a{}^\gamma{}_\delta \Lambda^\delta{}_\beta + (\Lambda^{-1})^\alpha{}_\gamma D_a \Lambda^\gamma{}_\beta$. Let us now compare this structure with that in the gravitational case. The analog of the Yang-Mills connection is the equivalence class $\{D\}$. To specify a $\{D\}$, it is sufficient to give its action on a covector field l_a satisfying $l_a n^a = 1$, $D_{[a}l_{b]} = 0$ and $\mathscr{L}_n l_a = 0$. *In this sense*, the field l_a is the analog of a basis $e^\alpha{}_\alpha$. Geometrically, l_a defines a foliation of $\mathscr{I}$ by a one-parameter family of 2-spheres–as a covector field, l_a is normal to this family– which is mapped into itself by n^a. Hence it follows that any two such l_a and l'_a can be obtained from each other by a supertranslation. *In this sense*, the supertranslation group ST is the analog of the local gauge group G_L. Next, it is easy to check that, given a classical vacuum $\{\mathring{D}\}$, there exists a l_a such that[24] $\{\mathring{D}_a\}l_b = 0$ and that if l_a and l'_a are two permissible fields satisfying this condition, then l_a and l'_a are related by a translation. We are thus led to Theorem 2 in an alternate way: the quotient ST/T of supertranslations by translations acts simply and transitively on the collection of classical vacua. Thus, T plays the role of the global gauge group. Next, we can fix any one classical vacuum $\{\mathring{D}\}$ and label points $\{D\}$ of Γ by tensor fields γ_{ab}. Under the change of origin, $\{\mathring{D}\}\to\{\mathring{D}'\}$, we have $\gamma_{ab}\to\gamma_{ab}' = \gamma_{ab} + \mathring{D}_a\mathring{D}_b f$ where $\{\mathring{D}\}$ and $\{\mathring{D}'\}$ are related by the supertranslation fn^a.

Note, however, that the analogy is rather formal: The

bases $e^{\alpha}{}_{a}$, the global gauge group G, and the local gauge group G_L play a wide variety of roles in the Yang-Mills theory and only a few of these are played by the fields l_a, the translation group T and the supertranslation group ST. Thus, for instance, the field l_a cannot serve to reduce γ_{ab} to its components. More importantly, the detailed procedure by which one "gauges" field theories—i.e., passes from global gauge transformations to local ones, *performed at each point of space-time*—does not carry over. All these differences are important: we shall see in the next paper that the quanta which emerge from connections $\{D\}$ have spin 2, rather than 1, and so the two frameworks contain quite different information. Despite this, the formal analogy is useful in several ways. From a mathematical viewpoint, for example, one can see that, since T is abelian, in the present framework, one cannot hope to find "nontrivial" vacua analogous to those carrying nonzero topological quantum numbers in the Yang-Mills theory. From a physical viewpoint, the analogy adds an interesting facet to the enlargement of the translation subgroup to the supertranslation one which occurs in presence of gravitational radiation.

ACKNOWLEDGMENTS

Anne Magnon-Ashtekar and Michael Streubel provided many stimulating discussions in the initial stages of this work, and Ted Newman's probing questions led to a great deal of clarity in the final presentation. To all three, I am grateful.

APPENDIX A: RELATION TO THE NEWMAN–PENROSE FORMALISM

Fix a space-time $(\hat{M}, \hat{g}_{ab})$ which is asymptotically empty and flat at null infinity. Consider a conformal completion (M, g_{ab}) such that the induced q_{ab} on I is the lift to I of a unit 2-sphere metric on the space of generators. Then n^a generates a BMS time translation. Fix a cross section of I and obtain a foliation of I by translating this cross section along n^a. Introduce a coordinate u on I such that the one-parameter family of cross sections is labelled by $u = \text{const}$. Thus, on I, u satisfies $\mathcal{L}_n u = 1$. Denote by l^a the unique null vector field on I, orthogonal to these cross sections, which satisfies $g_{ab} l^a n^b = -1$. Finally, introduce a complex vector field m^a, tangential to the cross sections, satisfying $\mathcal{L}_n m^a = 0$, $m \cdot m = 0$, and $m \cdot \bar{m} = 1$. Then, $(n^a, l^a, m^a, \bar{m}^a)$ gives us a null tetrad at any point of I. Set $\sigma^0 = m^a m^b \nabla_a l_b$. ($\sigma^0$ is independent of the particular extension of l_b off I, chosen in its evaluation.) σ^0 is the asymptotic shear. $\mathcal{L}_n \sigma^0 \equiv N$ is called the Bondi news function. Finally, the ten components of the asymptotic Weyl curvature, K_{abcd}, are captured in five complex functions $\psi_4{}^0$, $\psi_3{}^0$, $\psi_2{}^0$, $\psi_1{}^0$, and $\psi_0{}^0$. Five of these ten quantities are completely determined by the shear σ^0:

$$\psi_4{}^0 = -\ddot{\bar{\sigma}}^0, \quad \psi_3{}^0 = \eth \dot{\bar{\sigma}}^0,$$
$$2IM\psi_2{}^0 = \bar{\sigma}^0 \dot{\sigma}^0 - \sigma^0 \dot{\bar{\sigma}}^0 + \eth^2 \sigma^0 - \eth^2 \bar{\sigma}^0, \tag{A1}$$

where the dot stands for $n^a \partial_a$. The remaining five components contain "longitudinal" information and are not captured in σ^0 alone. (For details, see Ref. 25).

Consider the pull-back $\underset{\_}{l}_a$ to I of the covector field l_a. Set $\sigma^0{}_{ab} = \underset{\_}{D}_a \underset{\_}{l}_b - \frac{1}{2} \underset{\_}{q}_{ab} \underset{\_}{q}^{mn} \underset{\_}{D}_m \underset{\_}{l}_n$. (Note that $\underset{\_}{D}_a \underset{\_}{l}_b = \underset{\_}{D}_{(a} \underset{\_}{l}_{b)}$ and that $\underset{\_}{q}^{mn} \underset{\_}{D}_m \underset{\_}{l}_n$ is well-defined because $\underset{\_}{n}^m \underset{\_}{D}_m \underset{\_}{l}_n = 0$ on I.) Clearly, $\underset{\_}{\sigma}^0{}_{ab}$ contains the same information as σ^0 although it is independent of the choice of m^a. We shall now show that, together with l_a, $\underset{\_}{\sigma}^0_{ab}$ contains the same information as the element $\{D\}$ of Γ.

Define, on I, a symmetric connection $\underset{\_}{\mathring{D}}$ satisfying Eq. (7a) and the condition $\underset{\_}{\mathring{D}}_a l_b = 0$. From the discussion following Eq. (7a) it is clear that $\underset{\_}{\mathring{D}}$ is completely specified by these conditions. A direct calculation shows that $\underset{\_}{\mathring{D}}$ has trivial curvature whence $\{\underset{\_}{\mathring{D}}\}$ is a classical vacuum. (The four-parameter family of cross sections obtained from $u = 0$ by the action of BMS translations is shear-free w.r.t. the connections in $\{\underset{\_}{\mathring{D}}\}$. As one might expect, the Poincaré subgroup of the BMS group which leaves this family invariant is the same as that selected by $\{\underset{\_}{\mathring{D}}\}$ via Theorem 3.) Let us use this $\{\underset{\_}{\mathring{D}}\}$ as origin. Then, any element $\{\underset{\_}{D}\}$ of Γ can be labelled by a tensor field γ_{ab} satisfying $\gamma_{ab} = \gamma_{(ab)}$, $\gamma_{ab} n^b = 0$, and $\gamma_{ab} q^{ab} = 0$. Consider the connection $\underset{\_}{D}$ induced on I by ∇. We have $(\underset{\_}{D}_a - \underset{\_}{\mathring{D}}_a) \underset{\_}{l}_b \equiv \underset{\_}{D}_a \underset{\_}{l}_b = \Sigma_{ab} \underset{\_}{n}^c \underset{\_}{l}_c \equiv \Sigma_{ab}$, whence $\{D\} - \{\mathring{D}\}$ is characterized by the trace-free part of Σ_{ab}. Thus, $\{D\}$ is labelled by $\underset{\_}{\gamma}_{ab}$ defined by $\underset{\_}{\gamma}_{ab} = \underset{\_}{D}_a \underset{\_}{l}_b - \frac{1}{2} \underset{\_}{q}_{ab} \underset{\_}{q}^{mn} \underset{\_}{D}_m \underset{\_}{l}_n$. Hence $\underset{\_}{\gamma}_{ab} = \underset{\_}{\sigma}^0_{ab}$: $\{D\}$ and $\underset{\_}{\sigma}^0_{ab}$–or, equivalently, $\underset{\_}{\sigma}^0$–contain identical information. Next, since $N = \mathcal{L}_n \sigma^0$, it follows that $N = m^a m^b N_{ab}$. Finally, Eqs. (A1) are equivalent to Eqs. (3) and (5).

Thus, by choosing a cross section of I, Newman and Penrose first introduce an origin in Γ and then, using this origin, represent the connections, news tensors, and asymptotic curvatures in terms of spin and boost weighted scalars. The choice of origin, however, is not a natural one. For example, under a supertranslation, the origin is shifted and the scalars undergo transformations reflecting this change. In particular, the vector space structure that the space of shears appears to have is *not* a natural one: The notion of zero shear fails to be invariant under supertranslations. Hence, the choice of cross section is similar to the choice of a gauge in Yang–Mills theory; it simplifies many computations but complicates the analysis of conceptual issues since it introduces auxiliary structure which is not naturally available. (Thus, for example, the use of shears σ^0 as the basic dynamical variable had led to an incorrect expression for the symplectic structure; it is rather easy to overlook the fact that the vector space structure on the space of shears is illusory.)

In the framework presented in Sec. III, gauge makes its appearance via transformations $D \to \tilde{D}$ where $\tilde{D}_a K_b = D_a K_b - f q_{ab} n^c K_c$. It is this freedom that led us to equivalence classes $\{D\}$. What is the status of this freedom in the Newman–Penrose formalism? Since this freedom arises from that of conformal rescalings $g_{ab} \to \omega^2 g_{ab}$ (with $\omega = 1$ on I but $\nabla_a \omega \neq 0$ on I), it persists in the Newman–Penrose formalism as we have summarized it here. However, it can be and often is eliminated by requiring that the conformal factor Ω be so chosen that not only should q_{ab} be a unit 2-sphere metric but l_a be divergence free on I. One can use a similar technique on $\mathscr{I}$. We could have fixed a covector field l_a on $\mathscr{I}$ satisfying $D_{[a} l_{b]} = 0$, $\mathcal{L}_n l_a = 0$, and $l_a n^a = 1$ and permitted only those connections D in C which satisfy $(D_a l_b) q^{ab} = 0$. It is easy to verify that there exists one and

only one connection D in each equivalence $\{D\}$ in Γ which satisfies this requirement. This "gauge-fixing" procedure was not used in the main body of the paper only for aesthetic reasons.

APPENDIX B: EXTENSION TO ELECTROVAC SPACE-TIMES

A space–time $(\hat{M}, \hat{g}_{ab})$ will be said to be asymptotically electrovac and flat at null infinity if it satisfies conditions (i), (ii), and (iii) of the definition in Sec. II, as well as the following weakened version of (iv):

(iv') There exists a neighborhood N of I in M such $\hat{g}_{ab}$ satisfies the Einstein's equation with a Maxwell field $\hat{F}_{ab}$ as a source and $\hat{F}_{ab}$ admits a smooth limit to I.

Conditions (i), (ii), (iii), (iv') have the following consequences. Since $\hat{F}_{ab}$ admits a limit to I, its stress-energy tensor vanishes to order four in the sense of Geroch.[10] Hence, I is again a null surface with the same universal structure as in Sec. II and the Weyl tensor C_{abcd} of g_{ab} vanishes on I. Hence, we introduce the fields $\underset{\sim}{K}^{ab}$ and $*\underset{\sim}{K}^{ab}$ on I in terms of $K^{abcd} := \Omega^{-1} C^{abcd}$. The connection ∇ compatible with g_{ab} induces a connection D satisfying Eq. (1) and it Riemann tensor, R_{abcd}, is again given in terms of $\underset{\sim}{S}^{a}{}_{b}$ by Eq. (3). Finally, we can introduce the news tensor N_{ab} which satisfies Eq. (14). Because of presence of sources, however, the second of Eqs. (5) is modified. We have, instead,

$$D_b \underset{\sim}{K}^{ab} = -4\underset{\sim}{n}^a \underset{\sim}{n}^m \underset{\sim}{n}^n \underset{\sim}{L}_{mn}, \tag{B1}$$

where $\underset{\sim}{L}_{mn}$ is the pullback to I of $4\pi G\Omega^{-2}(\hat{F}_{ma}\hat{F}_{nb} + *\hat{F}_{ma} *\hat{F}_{nb})\hat{g}^{ab}$. [The first and third of Eqs. (5) remain unaltered.] In addition, via pull-back, we acquire two fields $\hat{F}_{ab}$ and $*\hat{F}_{ab}$ on I. These satisfy the equations

$$D_{[a}\underset{\sim}{F}_{bc]} = 0, \quad D_{[a} *\underset{\sim}{F}_{bc]} = 0, \tag{B2}$$
$$*\underset{\sim}{F}_{ab}\underset{\sim}{n}^b = \tfrac{1}{2}\underset{\sim}{q}_{am}\underset{\sim}{\epsilon}^{mcd}\underset{\sim}{F}_{cd}$$

and

$$\underset{\sim}{F}_{ab}\underset{\sim}{n}^b = -\tfrac{1}{2}\underset{\sim}{q}_{am}\underset{\sim}{\epsilon}^{mcd} *\underset{\sim}{F}_{cd}.$$

[Note that, since the differential equations in (B2) involve only a curl, it is only Eq. (B1) that exhibits the presence of a coupling between the gravitational and the electromagnetic fields on I.] Let us restrict ourselves to the situation in which there exists no magnetic charges in $\hat{M}$. Then, one can introduce, in a neighborhood of I, *a global vector potential* $\hat{A}_a$. Denote by $\underset{\sim}{A}_a$ the pullback to I of $\hat{A}_a$. The gauge freedom in $\underset{\sim}{A}_a$ can be partially eliminated by demanding that it satisfy $\underset{\sim}{A}_a \underset{\sim}{n}^a = 0$. Consider equivalence classes $\{A\}$ of such fields where $\underset{\sim}{A}_a \approx \underset{\sim}{A}'_a$ if $\underset{\sim}{A}'_a - \underset{\sim}{A}_a = D_a f$ with $\mathcal{L}_n f = 0$. Each $\{\underset{\sim}{A}_a\}$ has two components which represent the two electromagnetic radiative modes. Since $\underset{\sim}{F}_{ab} = D_{[a}\underset{\sim}{A}_{b]}$, $\{\underset{\sim}{A}_b\}$ determines $\underset{\sim}{F}_{ab}$, and hence, via Eq. (16), also $*\underset{\sim}{F}_{ab}\underset{\sim}{n}^b$. However, it fails to determine the component of $*\underset{\sim}{F}_{ab}$ carrying information about the "longitudinal mode." (Thus, $\{\underset{\sim}{A}_a\}$ is analogous to $\{D\}$, $\underset{\sim}{F}_{ab}$ to $*\underset{\sim}{K}^{ab}$ and $*\underset{\sim}{F}_{ab}$ to $\underset{\sim}{K}^{ab}$.) In terms of I, one can proceed as follows. The gravitational radiative modes can again be represented by equivalence classes $\{D\}$ of connections which lead to the fields N_{ab} and $*\underset{\sim}{K}^{ab}$. *The algebraic and differential equations on these fields remain unaltered.* The electromagnetic radiative modes can be represented by equivalence classes $\{\underset{\sim}{A}_a\}$ of covector fields on $\mathcal{I}$. Denote the space of these equivalence classes by Γ_M. Then, $\Gamma \cup \Gamma_M$ represents the space of Einstein-Maxwell radiative modes. Thus, as far as the radiative degrees are concerned, a complete decoupling occurs on $\mathcal{I}$. The situation is quite analogous in the Einstein-Yang-Mills case. Note, however, that the decoupling has not been introduced by hand; the classical theory itself predicts the occurrence of this simplification. We shall see in the next paper that this simplification plays a key role in the quantization procedure.

[1] A. Ashtekar, Phys. Rev. Lett. **46**, 573 (1981). The main results were also reported at the second Oxford Quantum Gravity Symposium.

[2] For details, see, e.g., A. Ashtekar and R. Geroch, Rep. Prog. Phys. **37**, 1211 (1974).

[3] As Penrose puts it, "if we remove life from Einstein's beautiful theory by steam-rollering it first to flatness and linearity, then we shall learn nothing from attempting to wave the magic wand of quantum theory over the resulting corpse"[R. Penrose, Gen. Rel. Grav. **7**, 31 (1976)].

[4] R. Schoen and S. T. Yau, Phys. Rev. Lett. **43**, 1459 (1979) and references contained therein.

[5] See, e.g., K. Kuchař, in *Proceedings of the Second Oxford Symposium on Quantum Gravity*, edited by C. J. Isham, R. Penrose, and D. Sciama (Oxford U. P., to appear).

[6] This idea is not new. It appeared in the literature already in the early sixties [see, in particular, R. K. Sachs, Phys. Rev. **128**, 2851 (1962), and A. Komar, Phys. Rev. **134**, B1430 (1964)] and was implicit in the work of R. Penrose, completed even before. More recent contributions in this broad direction came via the discovery of H-spaces by E. T. Newman and of nonlinear gravitons by R. Penrose. [See, e.g., M. Ko, M. Ludvigsen, and E. T. Newman, Phys. Rep. **71**, 51 (1981).]

[7] By a space-time $(\hat{M}, \hat{g}_{ab})$ we mean a c^∞ 4-manifold $\hat{M}$ equipped with a $\hat{g}_{ab}$ of signature $(-+++)$. Our conventions for curvature tensors are $\hat{\nabla}_{[a}\hat{\nabla}_{b]}K_c = \tfrac{1}{2}\hat{R}_{abc}{}^{d}K_d$, $\hat{R}_{ac} = \hat{R}_{abc}{}^{b}$ and $\hat{R} = \hat{g}^{ab}\hat{R}_{ab}$. The possibility of weakening of c^∞ requirement is being investigated in collaboration with A. Sen.

[8] This definition is taken from R. Geroch and G. T. Horowitz, Phys. Rev. Lett. **40**, 203 (1978).

[9] For extension to electrovac space-times, see Appendix B.

[10] R. Geroch, in *Asymptotic Structure of Space-Times*, edited by F. Esposito and L. Witten (Plenum, New York, 1977).

[11] Throughout this paper, I (or $\mathcal{I}$) will stand for "future *or* past null infinity."

[12] Note that we are *not* requiring the space-times to be asymptotically simple; space-times may, for example, admit event horizons. Hence, in general, we will obtain only a superscattering operator in the quantum description.

[13] In the actual construction of the superscattering operators, we will probably have to impose suitable conditions at i^0 as well in order to tie the structure of $\mathcal{I}^-$ to that of $\mathcal{I}^+$.

[14] B. G. Schmidt, M. Walker, and P. Sommers, Gen. Rel. Grav. **6**, 489 (1975).

[15] The result $R_{abcd} = R^0{}_{abcd}$ is an immediate consequence of Lemma 2.1.

[16] The news tensor N_{ab} has the same algebraic properties. However, just as in gauge theories the curvature tensor fails to determine the connection uniquely, N_{ab} fails to determine $\{D\}$ (and $*K^{ab}$) uniquely. Since we need derivative operators D to write various asymptotic differential equations, it is natural, as in gauge theories, to regard the connection as the basic variable.

[17] Since Γ has only two degrees of freedom, one may be tempted to call it the configuration space rather than the phase space. However, as the analogy with the Maxwell theory shows, it is indeed the phase space; the degrees of freedom are cut in half because of the use of null, rather than spacelike, surfaces.

[18] In the case of BMS translations, the expression reduces to the Bondi flux formula. For general BMS vector fields, several inequivalent local flux expressions are available in the literature. Among these, the expression obtained using (Γ, Ω) is the only one with the physically expected property of vanishing identically in Minkowski space. For details, see A. Ashtekar and M. Streubel, Proc. R. Soc. London Ser. A **376**, 585 (1981).

[19]The curvature cannot vanish identically because, for *any* connection D in C, $R_{abc}{}^{d}q_{de} = R^{0}{}_{abce}$, the lift to $\mathscr{F}$ of the curvature tensor on the space of generators and this space, being diffeomorphic to S^2, does not admit a flat connection.

[20]Note that $\mathring{\Sigma}_{ab}$ is not necessarily trace-free because D and D' have been fixed by the requirement $\mathring{S}_{a}{}^{b} = \mathring{S}'{}_{a}{}^{b} = \frac{1}{2}R^{0}\delta_{a}{}^{b}$ and $\mathring{\Sigma}_{ab}$ characterizes the difference between these specific connections and not just between $\{D\}$ and $\{D'\}$.

[21]Here, we are considering only the kinematic structure of the two theories Dynamically, of course, the theories are quite different since Einstein's Lagrangian is linear, rather than quadratic, in curvature.

[22]The formulation of Yang-Mills theory using Penrose's abstract index notation is discussed in A. Ashtekar, G. T. Horowitz, and A. Magnon-Ashtekar, "A generalization of tensor calculus and its application to physics," Gen. Rel. Grav. (in press).

[23]R. Penrose, in *Battelle Rencontres*, edited by C. DeWitt and J. A. Wheeler (Benjamin, New York, 1968).

[24]I.e., $D_a l_b$ is proportional to q_{ab}.

[25]E. T. Newman and R. Penrose, Proc. R. Soc. London Ser. A **305**, 175 (1968).

On a completely symmetric choice of space–time coordinates

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(Received 15 August 1980; accepted for publication 24 October 1980)

It is shown that for a wide class of space–times the four coordinates may be chosen in a completely symmetric way. Such symmetric coordinates have the same causal nature in that they are all measured by the same type of prescription involving clocks and/or measuring rods. In these coordinate systems the metric tensor is invariant with respect to any permutation of the coordinate labels 0, 1, 2, 3.

PACS numbers: 04.20.Cv

1. INTRODUCTION

The object of this present paper is to exhibit classes of symmetric coordinate systems applicable to a wide variety of metrics of four-dimensional Riemannian space–times of the usual signature. We focus attention initially, in Secs. 2–8, on the Minkowski space of special relativity, and then extend the results to general relativity in Sec. 9.

In Minkowski space–time the usual coordinates x^0, x^1, x^2, x^3 display asymmetry between x^0 and the spatial variables x^1, x^2, x^3. The latter three are similar in nature, being in principle obtained using meter sticks, but x^0 is measured on clocks. The origin of the difference is of course the causal structure of space-time, timelike and spacelike intervals being manifestly quite different. The subterfuge of taking an imaginary coordinate $x^4 = ix^0$ does not remove the asymmetry—we cannot use a meter stick to measure x^4 any more than we could x^0! It is misleading to try to disguise the difference between timelike and spacelike intervals which is endemic to our world. However it is important to realize that it is precisely here, in the different nature of the two types of intervals, that the asymmetry belongs. The point of this paper is that the *coordinates* do not necessarily have to display that asymmetry but may be chosen in a completely symmetric way.

In Sec. 2 we introduce coordinates ξ^κ which are real linear combinations of the Minkowski coordinates x^κ. All four coordinates ξ^κ are of the same causal nature in the following sense: Let each of the coordinates ξ^κ be incremented in turn to $\xi^\kappa + d\xi^\kappa$ leaving the other three coordinates unchanged. Then the four intervals $(\xi^0,\xi^1,\xi^2,\xi^3)$ to $(\xi^0 + d\xi^0, \xi^1,\xi^2,\xi^3)$, $(\xi^0,\xi^1,\xi^2,\xi^3)$ to $(\xi^0,\xi^1 + d\xi^1,\xi^2,\xi^3)$, and so on, are all timelike, null or spacelike. (Which of the three possibilities occurs depends on the choice of two free parameters ζ and ν in the transformation.) Further, any permutation of the new coordinate labels leaves the metric tensor unchanged. This is in contrast to the Minkowski coordinates where, for example, $x'^0 = x^1$, $x'^1 = x^2$, $x'^2 = x^0$, $x'^3 = x^3$ is not a Lorentz transformation. Permutation symmetry is restricted to the three Minkowski spatial variables.

The possibility of realization of our goal of coordinate symmetry is suggested by the recent results of Patera, Saint-Aubin, and Zassenhaus.[1] These authors show how to construct the finite subgroups of the generalized Lorentz groups $O(p, q)$. In particular they list all the finite subgroups of the ordinary Lorentz group O(3, 1) and prove the following surprising lemma: Every finite subgroup of O(3, 1) is an O(3,1) conjugate of a subgroup of the orthogonal group O(4). In other words, given a finite set of Lorentz matrices L_i which together form a group under multiplication, then there exists a Lorentz matrix Y such that the matrices YL_iY^{-1} constitute a subgroup of O(4). The main result of Patera *et al.* which concerns us here is the existence of finite subgroups of O(3, 1) which are isomorphic to the symmetric group S_4, the group of permutations on four objects. These are the groups denoted by those authors $\langle \pm R'_2, R'_3\rangle$, $\langle R'_2 \oplus (-1), R'_3\rangle$ and $\langle -I_4 R'_2, R'_3\rangle$. Each of these groups is a set of 24 Lorentz matrices which is a faithful, though reducible, representation of S_4. The group theoretical aspects will be elaborated in Secs. 6–8.

2. SYMMETRIC COORDINATES IN SPECIAL RELATIVITY

Our starting point is consideration of real symmetric 4×4 matrices of the type

$$g = \begin{bmatrix} a & b & b & b \\ b & a & b & b \\ b & b & a & b \\ b & b & b & a \end{bmatrix}, \tag{1}$$

which have only two independent real elements, the diagonal elements $g_{00} = g_{11} = g_{22} = g_{33} = a$ and the offdiagonal elements $g_{01} = g_{02} = g_{03} = g_{12} = g_{23} = g_{31} = b$. We seek to transform our Minkowski metric η (diagonal elements 1, -1, -1, -1) into the above form by a similarity transformation

$$g = S^T \eta S, \tag{2}$$

corresponding to a change of coordinates $x^\kappa \to \xi^\kappa$:

$$x = S\xi. \tag{3}$$

Here S is a real nonsingular 4×4 matrix with transpose S^T, and x and ξ denote the column vectors constructed from x^κ and ξ^κ respectively. Clearly the transformation (2) is possible only if g has the same signature as η, i.e., has one positive and three negative eigenvalues. By inspection, a complete linearly independent set of right eigenvectors of g is $\{\mathbf{e}_0, \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$

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$$\mathbf{e}_0 = \tfrac{1}{2}\begin{bmatrix}1\\1\\1\\1\end{bmatrix},\quad \mathbf{e}_1 = \tfrac{1}{2}\begin{bmatrix}1\\1\\-1\\-1\end{bmatrix},$$
$$\mathbf{e}_2 = \tfrac{1}{2}\begin{bmatrix}1\\-1\\1\\-1\end{bmatrix},\quad \mathbf{e}_3 = \tfrac{1}{2}\begin{bmatrix}1\\-1\\-1\\1\end{bmatrix}. \tag{4}$$

These are orthonormal with respect to the four-dimensional Euclidean metric. The corresponding eigenvalues are $a+3b, a-b, a-b, a-b$. Hence for (2) to be possible we must confine ourselves to the domain $a+3b>0, b>a$.

Let us write

$$a = \tfrac{1}{4}(\zeta^2 - 3\nu^2),\quad b = \tfrac{1}{4}(\zeta^2 + \nu^2), \tag{5}$$

so that the eigenvalues are $\zeta^2, -\nu^2, -\nu^2, -\nu^2$. By definition ζ and ν are taken real and nonzero, but allowed to be either positive or negative. We now define a symmetric orthogonal matrix $Q\in O(4)$,

$$Q = [\mathbf{e}_0\mathbf{e}_1\mathbf{e}_2\mathbf{e}_3] = \tfrac{1}{2}\begin{bmatrix}1&1&1&1\\1&1&-1&-1\\1&-1&1&-1\\1&-1&-1&1\end{bmatrix}, \tag{6}$$

and a diagonal matrix Λ,

$$\Lambda = \begin{bmatrix}\zeta&&&\\&-\nu&&\\&&-\nu&\\&&&-\nu\end{bmatrix}. \tag{7}$$

Clearly Q is its own inverse and diagonalizes g:

$$QgQ = \Lambda\eta\Lambda. \tag{8}$$

Thus we obtain (2) with the identification $S = \Lambda Q$. The change of coordinates (3) is then

$$\begin{aligned}x^0 &= \tfrac{1}{2}\zeta(\xi^0 + \xi^1 + \xi^2 + \xi^3),\\ x^1 &= -\tfrac{1}{2}\nu(\xi^0 + \xi^1 - \xi^2 - \xi^3),\\ x^2 &= -\tfrac{1}{2}\nu(\xi^0 - \xi^1 + \xi^2 - \xi^3),\\ x^3 &= -\tfrac{1}{2}\nu(\xi^0 - \xi^1 - \xi^2 + \xi^3),\end{aligned} \tag{9}$$

with inverse relations

$$\begin{aligned}\xi^0 &= \tfrac{1}{2}x^0/\zeta - \tfrac{1}{2}(x^1 + x^2 + x^3)/\nu,\\ \xi^1 &= \tfrac{1}{2}x^0/\zeta - \tfrac{1}{2}(x^1 - x^2 - x^3)/\nu,\\ \xi^2 &= \tfrac{1}{2}x^0/\zeta - \tfrac{1}{2}(-x^1 + x^2 - x^3)/\nu,\\ \xi^3 &= \tfrac{1}{2}x^0/\zeta - \tfrac{1}{2}(-x^1 - x^2 + x^3)/\nu.\end{aligned} \tag{10}$$

The Jacobian determinant of the transformation is $|S| = \zeta\nu^3$. (Note that Q is an improper rotation.) Hence if we wish to preserve the orientation of coordinates then ζ and ν must be chosen of the same sign.

To summarize, what we have established is the following. Given any two real nonzero numbers ζ, ν, either positive or negative, the transformation of coordinates $x^\kappa \to \xi^\kappa$ given by (9) and (10) transforms the metric tensor to the form (1) with

$$\begin{aligned}g_{\lambda\mu} &= \tfrac{1}{4}(\zeta^2 - 3\nu^2) \text{ if } \lambda = \mu,\\ &= \tfrac{1}{4}(\zeta^2 + \nu^2) \text{ if } \lambda \neq \mu.\end{aligned} \tag{11}$$

The eigenvalues of the matrix $g = [g_{\lambda\mu}]$ are $\zeta^2, -\nu^2, -\nu^2, -\nu^2$. The contravariant metric components are

$$\begin{aligned}g^{\lambda\mu} &= \tfrac{1}{4}(\zeta^{-2} - 3\nu^{-2}) \text{ if } \lambda = \mu,\\ &= \tfrac{1}{4}(\zeta^{-2} + \nu^{-2}) \text{ if } \lambda \neq \mu.\end{aligned} \tag{12}$$

3. CAUSAL NATURE OF THE COORDINATES ξ

Let us introduce four basis vectors $\mathbf{u}_{(\alpha)}$, $\alpha = 0, 1, 2, 3$, whose contravariant components in the ξ-system are defined to be[2]

$$u'^{\lambda}_{(\alpha)} = \delta^\lambda_\alpha. \tag{13}$$

An increment of coordinate α keeping all other coordinates fixed then corresponds to a displacement vector protional to $\mathbf{u}_{(\alpha)}$. We must distinguish five cases, according to the causal nature of the $\mathbf{u}_{(\alpha)}$:

(i) $\zeta > 3^{\frac{1}{2}}\lvert\nu\rvert$,	future timelike,
(ii) $\zeta = 3^{\frac{1}{2}}\lvert\nu\rvert$,	future null,
(iii) $-3^{\frac{1}{2}}\lvert\nu\rvert < \zeta < 3^{\frac{1}{2}}\lvert\nu\rvert$,	spacelike,
(iv) $\zeta = -3^{\frac{1}{2}}\lvert\nu\rvert$,	past null,
(v) $\zeta < -3^{\frac{1}{2}}\lvert\nu\rvert$,	past timelike.

Thus in case (i) *all four* coordinates ξ^λ are future timelike, in case (ii) *all* are future null, in case (iii) *all* are spacelike and so on. Hence all four coordinates are to be measured by similar prescriptions, be it by clocks or meter sticks or combinations of both types of device. An interesting implication of case (ii) is that any vector may be written as a linear superposition of four fixed future null vectors.

Similar results with $\zeta \to \zeta^{-1}, \nu \to \nu^{-1}$ pertain if we examine the causal nature of vectors perpendicular to the hyperplanes $\xi^\kappa = \text{const}$. We are then considering the four vectors $\mathbf{v}^{(\alpha)}$ whose covariant components in the ξ-system are

$$v'^{(\alpha)}_\lambda = \delta^\alpha_\lambda. \tag{14}$$

The results on the causal character of the basis vectors $\mathbf{u}_{(\alpha)}$ and $\mathbf{v}^{(\alpha)}$ are collated in Table I.

TABLE I. Columns two and three give the causal nature of the basis vectors $\mathbf{u}_{(\alpha)}$ and $\mathbf{v}^{(\alpha)}$ for the various domains of the transformation parameters ζ, ν. The vectors $\mathbf{u}_{(\alpha)}$ and $\mathbf{v}^{(\alpha)}$, defined by (13) and (14), are proportional to displacements along the ξ axes, and perpendicular to the hyperplanes $\xi^\kappa = \text{const}$, respectively.

Parameter domain	$\mathbf{u}_{(\alpha)}$	$\mathbf{v}^{(\alpha)}$
$\zeta < -3^{\frac{1}{2}}\lvert\nu\rvert$	past timelike	spacelike
$\zeta = -3^{\frac{1}{2}}\lvert\nu\rvert$	past null	spacelike
$-3^{\frac{1}{2}}\lvert\nu\rvert < \zeta < -3^{-\frac{1}{2}}\lvert\nu\rvert$	spacelike	spacelike
$\zeta = -3^{-\frac{1}{2}}\lvert\nu\rvert$	spacelike	past null
$-3^{-\frac{1}{2}}\lvert\nu\rvert < \zeta < 0$	spacelike	past timelike
$0 < \zeta < 3^{-\frac{1}{2}}\lvert\nu\rvert$	spacelike	future timelike
$\zeta = 3^{-\frac{1}{2}}\lvert\nu\rvert$	spacelike	future null
$3^{-\frac{1}{2}}\lvert\nu\rvert < \zeta < 3^{\frac{1}{2}}\lvert\nu\rvert$	spacelike	spacelike
$\zeta = 3^{\frac{1}{2}}\lvert\nu\rvert$	future null	spacelike
$\zeta > 3^{\frac{1}{2}}\lvert\nu\rvert$	future timelike	spacelike

4. SPECIAL CASES

In this section we consider four special cases which typify the parameter domains of Table I.

A. $u_{(\alpha)}$ and $v^{(\alpha)}$ both spacelike

Of particular interest is the parameter set $\zeta = \nu = 1$, for with these values $g = [g_{\lambda\mu}]$ and $g^{-1} = [g^{\lambda\mu}]$ take the same numerical values.

$$g = g^{-1} = \tfrac{1}{2}\begin{bmatrix} -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \end{bmatrix}. \tag{15}$$

B. $u_{(\alpha)}$ spacelike and $v^{(\alpha)}$ future null

$$\zeta = 1, \quad \nu = 3^{\frac{1}{2}},$$

$$g = \begin{bmatrix} -2 & 1 & 1 & 1 \\ 1 & -2 & 1 & 1 \\ 1 & 1 & -2 & 1 \\ 1 & 1 & 1 & -2 \end{bmatrix},$$

$$g^{-1} = \tfrac{1}{3}\begin{bmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix}. \tag{16}$$

C. $u_{(\alpha)}$ future null, $v^{(\alpha)}$ spacelike

$$\zeta = 1, \quad \nu = 3^{-\frac{1}{2}}.$$

The metric tensor is as in (16) with g and g^{-1} interchanged.

D. $u_{(\alpha)}$ future timelike, $v^{(\alpha)}$ spacelike

$$\zeta = (11)^{\frac{1}{2}}, \quad \nu = 1,$$

$$g = \begin{bmatrix} 2 & 3 & 3 & 3 \\ 3 & 2 & 3 & 3 \\ 3 & 3 & 2 & 3 \\ 3 & 3 & 3 & 2 \end{bmatrix},$$

$$g^{-1} = \tfrac{1}{11}\begin{bmatrix} -8 & 3 & 3 & 3 \\ 3 & -8 & 3 & 3 \\ 3 & 3 & -8 & 3 \\ 3 & 3 & 3 & -8 \end{bmatrix}. \tag{17}$$

5. LORENTZ TRANSFORMATIONS

If $L \in O(3, 1)$ we may pass from one inertial set of coordinates x^κ to another set x'^κ via $x' = Lx$. The corresponding change $\xi^\kappa \to \xi'^\kappa$, for a fixed choice of ζ, ν, will be

$$\xi' = M\xi, \tag{18}$$

where $M = Q\Lambda^{-1}L\Lambda Q$. Clearly the set $M(\zeta, \nu)$ of all such matrices M is a group isomorphic to O(3, 1). Alternatively $M(\zeta, \nu)$ is the group composed of all matrices M satisfying

$$M^T g M = g, \tag{19}$$

with g given by (11).

6. PERMUTATION SYMMETRY

A. Permutations of coordinates

Let us consider the result of permuting the coordinate labels 0, 1, 2, 3, in the ξ-coordinate system. We adopt the cycle notation for permutations. For example, (123) $\{\xi^\kappa\}$ will mean the coordinate transformation $\xi'^0 = \xi^0, \xi'^2 = \xi^1$, $\xi'^3 = \xi^2, \xi'^1 = \xi^3$. It is sufficient to consider the effect of, say, the two elements (01) and (123) since all 24 permutations of S_4 may be generated as products with these two elements as factors.

If $P \in S_4$, then the transformation $P\{\xi^\kappa\}$ leaves the metric tensor unchanged. It follows that there must be a finite subgroup of matrices $M \in M(\zeta, \nu)$ which are a representation of S_4. The correspondence is clearly

$$(01) \to \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix},$$

$$(123) \to \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \tag{20}$$

and so on. If we now generate the Lorentz matrices corresponding to (02) and (123) by the prescription $L = \Lambda Q M Q \Lambda^{-1}$ we obtain the matrices designated $-R'_2$ and R'_3 by Patera *et al.*[3] Thus the symmetry of our formalism under permutations of the coordinates ξ^κ corresponds to the finite subgroup of O(3, 1) denoted by those authors $\langle -R'_2, R'_3 \rangle$, which is isomorphic to S_4.

B. Symmetric functions of the coordinates

It is instructive to examine the functions

$$s_n = \sum_{\lambda=0}^{3} (\xi^\lambda)^n, \quad n = 1, 2, 3, \ldots,$$

which are completely symmetric in all four coordinates. Expressed in terms of the Minkowski coordinates with the aid of (10) the first three such functions are

$$\begin{aligned} s_1 &= 2\zeta^{-1}x^0, \\ s_2 &= \zeta^{-2}(x^0)^2 + \nu^{-2}r^2, \\ s_3 &= \tfrac{1}{2}\zeta^{-3}(x^0)^3 + \tfrac{3}{2}\zeta^{-1}\nu^{-2}x^0r^2 - 3\nu^{-3}x^1x^2x^3, \end{aligned} \tag{21}$$

where

$$r^2 = (x^1)^2 + (x^2)^2 + (x^3)^2.$$

Hence x^0, r and $x^1x^2x^3$ are completely symmetric functions of the ξ^λ. This result will be of significance in Sec. 9, where we extend out results to general relativity.

C. Coordinate functions belonging to the representations of S_4

The properties of the irreducible representations S_4 are summarized in the Appendix. The five representations may be labelled according to the partitions of the number 4, [4], [31], [22], [211], [1111], having dimensions respectively, 1, 3, 2, 3, 1. The symmetric functions (21) belong to the symmetric representation [4]. We may also construct multinomials in the coordinates which belong to the rows of the other representations. Such functions, up to degree 2, are:

(i) belonging to [31]:

$$f_1 = \xi^0 + \xi^1 - \xi^2 - \xi^3 = -2\nu^{-1}x^1,$$
$$f_2 = \xi^0 - \xi^1 + \xi^2 - \xi^3 = -2\nu^{-1}x^2,$$
$$f_3 = \xi^0 - \xi^1 - \xi^2 + \xi^3 = -2\nu^{-1}x^3;$$
$$f_1' = (\xi^0 + \xi^1)^2 - (\xi^2 + \xi^3)^2 = -4(\zeta\nu)^{-1}x^0x^1,$$
$$f_2' = (\xi^0 + \xi^2)^2 - (\xi^3 + \xi^1)^2 = -4(\zeta\nu)^{-1}x^0x^2,$$
$$f_3' = (\xi^0 + \xi^3)^2 - (\xi^1 + \xi^2)^2 = -4(\zeta\nu)^{-1}x^0x^3;$$
$$f_1'' = (\xi^0 - \xi^1)^2 - (\xi^2 - \xi^3)^2 = 4\nu^{-2}x^2x^3,$$
$$f_2'' = (\xi^0 - \xi^2)^2 - (\xi^3 - \xi^1)^2 = 4\nu^{-2}x^3x^1,$$
$$f_3'' = (\xi^0 - \xi^3)^2 - (\xi^1 - \xi^2)^2 = 4\nu^{-2}x^1x^2.$$

(ii) belonging to [22]:

$$g_1 = 3^{-\frac{1}{2}}[(\xi^0 - \xi^2)(\xi^1 - \xi^3) + (\xi^0 - \xi^1)(\xi^2 - \xi^3)],$$
$$= \nu^{-2}3^{-\frac{1}{2}}[(x^1)^2 + (x^2)^2 - 2(x^3)^2],$$
$$g_2 = (\xi^0 - \xi^3)(\xi^1 - \xi^2) = \nu^{-2}[(x^1)^2 - (x^2)^2].$$

To construct functions belonging to [211] and [1111], one has to go to multinomials of higher order.

7. THE TRANSFORMED SPINOR MATRICES

A. The Pauli matrices

Consider the Pauli matrices σ^λ, $\bar\sigma^\lambda$ defined by

$$\sigma^0 = \bar\sigma^0 = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix},$$
$$\sigma^1 = -\bar\sigma^1 = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix},$$
$$\sigma^2 = -\bar\sigma^2 = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix},$$
$$\sigma^3 = -\bar\sigma^3 = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{22}$$

They satisfy

$$\bar\sigma^\lambda = \epsilon(\sigma^\lambda)^*\epsilon^\dagger,$$
$$\bar\sigma^\lambda\sigma^\mu + \bar\sigma^\mu\sigma^\lambda = 2\eta^{\lambda\mu}, \tag{23}$$

where $\epsilon = \begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}$. Note $\epsilon^\dagger = \epsilon^{-1} = -\epsilon$. Let us transform to the ξ-system by the prescription $\sigma'^\lambda = (\partial\xi'^\lambda/\partial x^\kappa)\,\sigma^\kappa$, $\bar\sigma'^\lambda$ analogously. These transformed Pauli matrices will then satisfy equations of the form (23) with $\eta^{\lambda\mu}$ replaced by $g^{\lambda\mu}$. We find

$$\sigma'^0 = \tfrac{1}{2}\sigma^0/\zeta - \tfrac{1}{2}(\sigma^1 + \sigma^2 + \sigma^3)/\nu,$$
$$\sigma'^1 = \tfrac{1}{2}\sigma^0/\zeta - \tfrac{1}{2}(\sigma^1 - \sigma^2 - \sigma^3)/\nu,$$
$$\sigma'^2 = \tfrac{1}{2}\sigma^0/\zeta - \tfrac{1}{2}(-\sigma^1 + \sigma^2 - \sigma^3)/\nu. \tag{24}$$
$$\sigma'^3 = \tfrac{1}{2}\sigma^0/\zeta - \tfrac{1}{2}(-\sigma^1 - \sigma^2 + \sigma^3)/\nu.$$

The matrices $\bar\sigma'^\lambda$ are obtained by replacing ν by $-\nu$ in (24).

An interesting feature of σ'^λ and $\bar\sigma'^\lambda$ is that all eight matrices have the same eigenvalues $\frac{1}{2}(\zeta^{-1} \pm 3^{\frac{1}{2}}\nu^{-1})$. This follows readily by noting that $(\sigma^1 \pm \sigma^2 \pm \sigma^3)^2 = 3\sigma^0$. Hence any pair of these matrices is related by a similarity transformation. Contrast this symmetry with the situation in Minkowski coordinates where σ^0 has eigenvalues 1, 1 and σ^1, σ^2, σ^3 eigenvalues ± 1.

By explicit calculation, we find that the relevant similarity transformations are the representation matrices of the projective (doubly valued) representation Γ_6 of S_4 (see Appendix). For a permutation P the result is

$$P\{\sigma'^\lambda\} = \Gamma_6(P)\sigma'^\lambda\Gamma_6^\dagger(P) \quad \text{if } P \text{ is even},$$
$$= \Gamma_6(P)\bar\sigma'^\lambda\Gamma_6^\dagger(P) \quad \text{if } P \text{ is odd}. \tag{25}$$

Note that an odd permutation corresponds to an improper Lorentz transformation.

The signature of the matrices σ'^λ, $\bar\sigma'^\lambda$ is correlated with the causal nature of $\mathbf{v}^{(\alpha)}$ given in Table I. The matrices are positive definite, negative definite, indefinite or singular according as the $\mathbf{v}^{(\alpha)}$ are future timelike, past timelike, spacelike or null respectively.

B. The Pauli angular momentum matrices

The spinor infinitesimal generators for O(3, 1) are

$$s^{\lambda\mu} = \tfrac{1}{4}i(\bar\sigma^\lambda\sigma^\mu - \bar\sigma^\mu\sigma^\lambda),$$

taking the values

$$(s^{23}, s^{31}, s^{12}) = -i(s^{01}, s^{02}, s^{03}) = \tfrac{1}{2}(\sigma^1, \sigma^2, \sigma^3).$$

The components in the ξ-system,

$$s'^{\lambda\mu} = \tfrac{1}{4}i(\bar\sigma'^\lambda\sigma'^\mu - \bar\sigma'^\mu\sigma'^\lambda),$$

are

$$s'^{23} = \tfrac{1}{4}i(\zeta\nu)^{-1}(\sigma^2 - \sigma^3) + \tfrac{1}{4}\nu^{-2}(\sigma^2 + \sigma^3),$$
$$s'^{01} = \tfrac{1}{4}i(\zeta\nu)^{-1}(\sigma^2 + \sigma^3) + \tfrac{1}{4}\nu^{-2}(\sigma^2 - \sigma^3),$$

with the other components being obtained by cyclic interchange of 1, 2, 3.

The eigenvalues of all the matrices $s'^{\lambda\mu}$ are $\pm\nu^{-1}[\frac{1}{8}(\nu^{-2} - \zeta^{-2})]^{\frac{1}{2}}$ which are purely real, zero or purely imaginary according as $|\zeta| \gtrless |\nu|$. This contrasts with the situation for the Minkowski generators where s^{23}, s^{31}, and s^{12} have the real eigenvalues $\pm\frac{1}{2}$ and s^{01}, s^{02}, s^{03} the imaginary eigenvalues $\pm\frac{1}{2}i$. Note that if $|\zeta| = |\nu|$, as in (15), then all eigenvalues of $s'^{\lambda\mu}$ are zero so that the matrices cannot then be diagonalized.

The permutation symmetry again involves Γ_6:

$$P\{s'^{\lambda\mu}\} = \Gamma_6(P)s'^{\lambda\mu}\Gamma_6^\dagger(P) \quad \text{if } P \text{ is even},$$
$$= \Gamma_6(P)\epsilon(s'^{\lambda\mu})^*\epsilon\Gamma_6^\dagger(P) \quad \text{if } P \text{ is odd}.$$

In Sec. 7 we have focused attention on the contravariant components of the Pauli matrices. Similar results hold for the covariant components σ'_λ, $\bar{\sigma}'_\lambda$, $s'_{\lambda\mu}$ with $\zeta \to \zeta^{-1}$, $\nu \to \nu^{-1}$.

8. THE TRANSFORMED DIRAC MATRICES

A. The matrices γ^λ and α^λ

Let us adopt the following representation for the Dirac matrices γ^λ, α^λ, β, partitioned into 2×2 submatrices:

$$\gamma^0 = \beta = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix},$$

$$\gamma^k = \begin{pmatrix} 0 & \sigma^k \\ -\sigma^k & 0 \end{pmatrix}, \quad k = 1, 2, 3,$$

$$\alpha^0 = \begin{pmatrix} I & 0 \\ 0 & I \end{pmatrix},$$

$$\alpha^k = \begin{pmatrix} 0 & \sigma^k \\ \sigma^k & 0 \end{pmatrix}, \quad k = 1, 2, 3.$$

They satisfy

$$\begin{aligned} &\gamma^\lambda\gamma^\mu + \gamma^\mu\gamma^\lambda = 2\eta^{\lambda\mu}, \\ &(\gamma^\lambda)^\dagger = \beta\gamma^\lambda\beta, \\ &(\alpha^\lambda)^\dagger = \alpha^\lambda = \beta\gamma^\lambda. \end{aligned} \tag{26}$$

If we transform γ^λ and α^λ as if they were contravariant vectors then the transformed components γ'^λ and α'^λ satisfy (26) with $\eta^{\lambda\mu}$ replaced by $g^{\lambda\mu}$. These matrices are

$$\gamma'^0 = \tfrac{1}{2}\begin{bmatrix} I/\zeta & -(\sigma^1+\sigma^2+\sigma^3)/\nu \\ (\sigma^1+\sigma^2+\sigma^3)/\nu & -I/\zeta \end{bmatrix},$$

$$\gamma'^1 = \tfrac{1}{2}\begin{bmatrix} I/\zeta & -(\sigma^1-\sigma^2-\sigma^3)/\nu \\ (\sigma^1-\sigma^2-\sigma^3)/\nu & -I/\zeta \end{bmatrix},$$

$$\alpha'^0 = \tfrac{1}{2}\begin{bmatrix} I/\zeta & -(\sigma^1+\sigma^2+\sigma^3)/\nu \\ -(\sigma^1+\sigma^2+\sigma^3)/\nu & I/\zeta \end{bmatrix},$$

$$\alpha'^1 = \tfrac{1}{2}\begin{bmatrix} I/\zeta & -(\sigma^1-\sigma^2-\sigma^3)/\nu \\ -(\sigma^1-\sigma^2-\sigma^3)/\nu & I/\zeta \end{bmatrix}.$$

The other components may be obtained by cyclic interchange of 1, 2, 3.

The eigenvalues of all the γ'^λ are $\pm\frac{1}{2}(\zeta^{-2} - 3\nu^{-2})^{\frac{1}{2}}$, and of α'^λ are $\frac{1}{2}(\zeta^{-1} \pm 3^{\frac{1}{2}}\nu^{-1})$, each eigenvalue being doubly degenerate. By direct calculation, or by first expressing γ'^λ and α'^λ in terms of σ'^λ and $\bar{\sigma}'^\lambda$ and applying (25), we find the permutation behavior to be

$$\begin{aligned} &P\{\gamma'^\lambda\} = D(P)\gamma'^\lambda D^\dagger(P), \\ &\text{with} \quad D(P) = \Gamma_6(P) \oplus \Gamma_7(P), \end{aligned} \tag{27}$$

and a similar result for α'^λ. (See Appendix.)

B. The Dirac angular momentum matrices

The appropriate infinitesimal generators for O(3, 1) are $J^{\lambda\mu} = \frac{1}{4}i(\gamma^\lambda\gamma^\mu - \gamma^\mu\gamma^\lambda)$, taking the values

$$J^{23} = \tfrac{1}{2}\begin{pmatrix} \sigma^1 & 0 \\ 0 & \sigma^1 \end{pmatrix}, \quad J^{01} = \tfrac{1}{2}i\begin{pmatrix} 0 & \sigma^1 \\ \sigma_1 & 0 \end{pmatrix},$$

and so on. The transformed components are

$$J'^{23} = \tfrac{1}{4}\begin{bmatrix} (\sigma^2+\sigma^3)/\nu^2 & i(\sigma^2-\sigma^3)/(\zeta\nu) \\ i(\sigma^2-\sigma^3)/(\zeta\nu) & (\sigma^2+\sigma^3)/\nu^2 \end{bmatrix},$$

$$J'^{01} = \tfrac{1}{4}\begin{bmatrix} (\sigma^2-\sigma^3)/\nu^2 & i(\sigma^2+\sigma^3)/(\zeta\nu) \\ i(\sigma^2+\sigma^3)/(\zeta\nu) & (\sigma^2-\sigma^3)/\nu^2 \end{bmatrix},$$

with the other components given by cyclic interchange.

The eigenvalues of all the $J'^{\lambda\mu}$ are $\pm\nu^{-1}[\frac{1}{8}(\nu^{-2} - \zeta^{-2})]^{\frac{1}{2}}$ as for the $s'^{\lambda\mu}$, except that each eigenvalue is doubly degenerate. Under permutations the transformation law is analogous to (27).

The eigenvalues of the covariant components γ'_λ, α'_λ, $J'_{\lambda\mu}$ may be obtained by the replacement $\zeta \to \zeta^{-1}$, $\nu \to \nu^{-1}$ in the above.

9. SYMMETRIC COORDINATES IN GENERAL RELATIVITY

A. General isotropic metric

Consider a metric of the isotropic type

$$ds^2 = A^2(t, r)dt^2 - B^2(t, r)(dx^2 + dy^2 + dz^2), \tag{28}$$

where A and B are arbitrary real functions of the "time" t and the "radial" coordinate $r = (x^2 + y^2 + z^2)^{1/2}$. Let us define new coordinates η^κ by analogy with (10):

$$\begin{aligned} \eta^0 &= \tfrac{1}{2}t/\zeta - \tfrac{1}{2}(x + y + z)/\nu, \\ \eta^1 &= \tfrac{1}{2}t/\zeta - \tfrac{1}{2}(x - y - z)/\nu, \\ \eta^2 &= \tfrac{1}{2}t/\zeta - \tfrac{1}{2}(-x + y - z)/\nu, \\ \eta^3 &= \tfrac{1}{2}t/\zeta - \tfrac{1}{2}(-x - y + z)/\nu, \end{aligned} \tag{29}$$

where ζ, ν may be any nonzero real numbers. Using (21), we see that t and r are completely symmetric functions of the η^κ:

$$\begin{aligned} &t = \tfrac{1}{2}\zeta s_1, \quad r^2 = \nu^2(s_2 - \tfrac{1}{4}s_1^2), \\ &s_1 = \eta^0 + \eta^1 + \eta^2 + \eta^3, \\ &s_2 = (\eta^0)^2 + (\eta^1)^2 + (\eta^2)^2 + (\eta^3)^2. \end{aligned} \tag{30}$$

With respect to the coordinates η^κ the metric components are

$$\begin{aligned} g'_{\lambda\mu} &= \tfrac{1}{4}(\zeta^2A^2 - 3\nu^2B^2) \quad \text{if } \lambda = \mu, \\ &= \tfrac{1}{4}(\zeta^2A^2 + \nu^2B^2) \quad \text{if } \lambda \neq \mu. \end{aligned} \tag{31}$$

This metric is now completely symmetric with respect to permutations of the coordinates η^κ. Its eigenvalues are ζ^2A^2, $-\nu^2B^2$, $-\nu^2B^2$, $-\nu^2B^2$.

B. The Friedmann–Robertson–Walker metric

As a special case we may consider the Friedmann–Robertson–Walker metric[4,5]

$$\begin{aligned} ds^2 &= dt^2 - R^2(t)(1 + \tfrac{1}{4}kr^2)^{-2}(dx^2 + dy^2 + dz^2) \\ &\equiv dt^2 - R^2(t)[(1 - k\bar{r}^2)^{-1}d\bar{r}^2 + \bar{r}^2d\Omega^2], \end{aligned}$$

where $\bar{r} = r(1 + \frac{1}{4}kr^2)^{-1}$ and k may be $\pm 1, 0$. The transformation (29) then yields the metric (31) with $A = 1$, $B = R(t)(1 + \frac{1}{4}kr^2)^{-1}$.

C. The Schwarzschild metric

Another interesting special case is the Schwarzschild metric[6]

$$ds^2 = (1 - \tfrac{1}{2}GM/r)^2(1 + \tfrac{1}{2}GM/r)^{-2}dt^2$$
$$- (1 + \tfrac{1}{2}GM/r)^4(dx^2 + dy^2 + dz^2)$$
$$\equiv (1 - 2GM/\bar{r})dt^2 - (1 - 2GM/\bar{r})^{-1}d\bar{r}^2 - \bar{r}^2 d\Omega^2,$$

where $\bar{r} = r(1 + \tfrac{1}{2}GM/r)^2$.

We now obtain (31) with
$A = (1 - \tfrac{1}{2}GM/r)/(1 + \tfrac{1}{2}GM/r)$, $B = (1 + \tfrac{1}{2}GM/r)^2$.

Note that the transformation (29) is only applicable outside the Schwarzschild radius $\bar{r} = 2GM$ or $r = \tfrac{1}{2}GM$. If $|\zeta| < 3^{\frac{1}{2}}|\nu|$ then the coordinates η^κ are spacelike for all $r > \tfrac{1}{2}GM$, but if $|\zeta| > 3^{\frac{1}{2}}|\nu|$ then there will exist a value of r at which the η^κ change from being spacelike to timelike as r increases through this value.

10. DISCUSSION

Merely changing from one set of coordinates to another, as we have done in this paper, will not alter the predictions of any satisfactory physical theory. Nevertheless the adoption of the coordinates ξ^κ does lead to some curious features. Consider, for example, a solution of the Klein–Gordon equation $g^{\lambda\mu}\partial^2\psi/\partial\xi^\lambda\partial\xi^\mu + \kappa^2\psi = 0$ in the plane wave form $\exp(-ik_\lambda\xi^\lambda)$. We have $g^{\lambda\mu}k_\lambda k_\mu = \kappa^2$ which may be solved for k_0 to give (if $g^{00} \neq 0$)

$$k_0 = (g^{00})^{-1}[-g^{0p}k_p \pm \{(g^{0p}g^{0q} - g^{00}g^{pq})k_p k_q + g^{00}\kappa^2\}^{1/2}], \tag{32}$$

where p, q are summed over 1, 2, 3. When $g^{00} = 0$, i.e., when $\zeta^2 = \nu^2/3$, (32) must be replaced by

$$k_0 = (\kappa^2 - g^{pq}k_p k_q)/(2g^{0s}k_s)$$
$$= (\tfrac{1}{2}\kappa^2\nu^2 - k_1k_2 - k_2k_3 - k_3k_1)/(k_1 + k_2 + k_3). \tag{33}$$

The two values of k_0 in (32) correspond to the two sheets of the momentum hyperboloid $g^{\lambda\mu}k_\lambda k_\mu = \kappa^2$. However when $\zeta^2 = \nu^2/3$ we obtain only the one value (33) for k_0. In this case the two sheets of the hyperboloid are distinguished by whether $k_1 + k_2 + k_3$ is positive or negative.

We turn now to the transformed Dirac equation

$$i\alpha'^\lambda\partial\psi/\partial\xi^\lambda = \kappa\beta\psi,$$

or equivalently

$$i\alpha'^0\partial\psi/\partial\xi^0 = -i\alpha'^p\partial\psi/\partial\xi^p + \kappa\beta\psi. \tag{34}$$

Let us restrict our attention to the parameter range $0 < \zeta < 3^{-\frac{1}{2}}\nu$. All the eigenvalues of α'^λ are then positive and we can find a positive definite Hermitian matrix T satisfying $T^{-2} = \alpha'^0$. Whence (34) takes the form

$$i\partial\phi/\partial\xi^0 = H\phi,$$

where

$$\phi = T^{-1}\psi,$$
$$H = -iT\alpha'^pT\partial/\partial\xi^p + \kappa T\beta T.$$

In this case the ξ^0-development of ϕ is generated by the Hermitian operator H which acts on the space of square-integrable 4-spinors $\phi(\xi^p)$. For this range of the parameters, ζ, ν, the coordinates ξ^κ, and in particular ξ^0, are spacelike but the hyperplanes $\xi^\kappa = \text{const}$ have timelike normals. The selection of ξ^0 as the "time" coordinate for Hamiltonian development is of course quite arbitrary. ξ^1, ξ^2, or ξ^3 would serve equally well.

Finally we may speculate on a possible application of our formalism to General Relativity. Metrics of the form (28) play a special role in Cosmology. We note that A and B are functions of t, r, or equivalently using (30), of the two simplest symmetric functions formed from η^κ, viz. s_1, s_2. The next simplest symmetric function is s_3, or equivalently xyz. Perhaps it might be fruitful to examine metrics of a form similar to (28) except that A, B would be taken functions of the three variables s_1, s_2, s_3, or equivalently, of t, r, xyz. Such metrics would in general be neither homogeneous or isotropic but would retain complete symmetry under permutations of the coordinates η^κ.

APPENDIX: THE REPRESENTATIONS OF THE SYMMETRIC GROUP S_4

The 24 permutations of S_4 may be grouped into five classes of conjugate elements[7]

$\mathscr{C}_1 = \{(0)\}$,

$\mathscr{C}_2 = \{(012), (023), (031), (021), (032), (013), (123), (132)\}$,

$\mathscr{C}_3 = \{(01)(23), (02)(31), (03)(12)\}$,

$\mathscr{C}_4 = \{(0123), (0231), (0312), (0132), (0213), (0321)\}$,

$\mathscr{C}_5 = \{(01), (02), (03), (23), (31), (12)\}$.

The five irreducible representations are labelled according to the partitions of the number 4, [4], [31], [22], [211], [1111] and have dimensions 1, 3, 2, 3, 1 respectively. It is sufficient to give the representation matrices for, say, the two elements (01) and (123) since any of the 24 permutations may be written as products with these elements as factors. We adopt the representations given by Cornwell[8]:

[4] $(01)\to 1$, $(123)\to 1$;

[31] $(01)\to \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{bmatrix}$,

$(123)\to \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$;

[22] $(01)\to \begin{pmatrix} -\frac{1}{2} & \frac{1}{2}3^{\frac{1}{2}} \\ \frac{1}{2}3^{\frac{1}{2}} & \frac{1}{2} \end{pmatrix}$,

$(123)\to \begin{pmatrix} -\frac{1}{2} & \frac{1}{2}3^{\frac{1}{2}} \\ -\frac{1}{2}3^{\frac{1}{2}} & -\frac{1}{2} \end{pmatrix}$;

[211] As for [31] with a change in sign for odd permutations;

[1111] $(01)\to -1$, $(123)\to 1$.

S_4 also possesses three projective representations, Γ_6, Γ_7, Γ_8 satisfying $\Gamma(P_1)\Gamma(P_2) = \pm\Gamma(P_1P_2)$. These are true representations of the 48 element double ochtahedral group[9] O^D which has a 2-1 homomorphism on to S_4. The representation matrices for the projective representations are given by Onodera and Okazaki.[10] We need only Γ_6 and Γ_7:

Γ_6 $(01)\to -2^{-\frac{1}{2}}i(\sigma^2 + \sigma^3)$,

$(123)\to\tfrac{1}{2}[1 - i(\sigma^1 + \sigma^2 + \sigma^3)]$,

with the Pauli matrices given by (22);

Γ_7 As for Γ_6 with a change of sign for (01), with (123) unchanged.

[1]J. Patera, Y. Saint-Aubin, and H. Zassenhaus, J. Math. Phys. **21**, 234 (1980).

[2]In general a prime will be used to distinguish tensor components referred to the ξ-system from the Minkowski components (unprimed). An exception is the metric tensor, whose components are denoted $g_{\lambda\mu}$ and $\eta_{\lambda\mu}$, respectively.

[3]Reference 1, Secs. IIIA and IIIB. Note that the symbol $-R_2'$ of Sec. IIIB means the 4×4 matrix $1\oplus(-I_3R_2')$ constructed from the 3×3 matrix R_2' of Sec. IIIA(d).

[4]A. Einstein, *The Meaning of Relativity* (Methuen, London, 1956), pp. 104–111.

[5]S. Weinberg, *Gravitation and Cosmology* (Wiley, New York, 1972), p. 412.

[6]Ref. 5, pp. 179–82.

[7]H. Boerner, *Representations of Groups* (North-Holland, Amsterdam, 1963), pp. 102–25, 184–213.

[8]J. F. Cornwell, *Group Theory and Electronic Energy Bands in Solids* (North-Holland, Amsterdam, 1969), pp. 21–5, 229–35. Identify $(01)\rightarrow IC_{2e}$, $(123)\rightarrow C_{3\delta}^{-1}$.

[9]Ref. 8, pp. 247–50.

[10]Y. Onodera and M. Okazaki, J. Phys. Soc. Japan **21**, 2400 (1966); Identify $(01)\rightarrow C_2'[011]$, $(123)\rightarrow C_3[111]$.

Memory function approach to nonlinear deterministic systems: An exact linear equation

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(Received 23 February 1981; accepted for publication 25 June 1981)

A set of nonlinear evolution equations is cast into an exact *linear* non-Markovian equation with the memory kernel reflecting the nonlinearity and coupling with irrelevant variables. The equation is deterministic in contrast to the generalized Langevin equation derived in a similar way. The solution to the nonlinear equations is expressed by a sum of exponential functions. A simple illustrative example is treated to show the effectiveness of the present approach.

PACS numbers: 05.20.Dd, 02.90. + p

1. INTRODUCTION

This paper is concerned with a system described by a set of coupled nonlinear evolution equations

$$\begin{cases} \dot{x}(t) = f(x(t), y_1(t), \ldots, y_n(t)), \\ \dot{y}_1(t) = g_1(x(t), y_1(t), \ldots, y_n(t)), \\ \dot{y}_n(t) = g_n(x(t), y_1(t), \ldots, y_n(t)) \end{cases} \tag{1a}$$

subject to given (i.e., fixed) initial condition

$$x(0) = a \neq 0, \qquad y_i(0) = b_i, \quad 1 \leqslant i \leqslant n, \tag{1b}$$

and aims at deriving from Eqs. (1a) and (1b) an exact linear non-Markovian equation of the following form:

$$\dot{x}(t) = \omega x(t) + \int_0^t \Lambda(t - t')x(t')\,dt'. \tag{2}$$

Here, x is the variable whose evolution is of interest to us, $y_1, \ldots, y_n$ are state variables necessary for the Markovian description (1a), and the overdot implies differentiation with respect to t.

The possibility of such an exact linearization has been suggested from our recent study on generalized Langevin equations.[1] We have shown that a set of coupled equations of motion can be converted into a linear non-Markovian Langevin equation; the *stochastic nature* of the equation arises from the fact that the initial values are not specified but *statistically distributed*. For the deterministic system (1a) with completely prescribed initial condition (1b), we shall show in the present paper that the stochastic force disappears and the generalized Langevin equation reduces to the deterministic Eq. (2).

The memory function $\Lambda(t)$ in Eq. (2) takes account of the nonlinearity and the coupling of x with the irrelevant variables $y_1, \ldots, y_n$, which have been eliminated in deriving Eq. (2); i.e., the memory function reflects all the complexity of the problem. Thus, the exact linear Eq. (2) does not imply that the exact solution to the nonlinear Eqs. (1a) is obtainable, and its usefullness depends entirely on an approximation made to the memory function. It is our *expectation* and the motivation of the present work that we can approximate the memory function more easily than $x(t)$ itself to obtain a result of the same quality. For instance, in a decaying system where $x(t) \to 0$ as $t \to \infty$, the memory function will decay more rapidly than $x(t)$, and is expected to be less sensitive to approximation. Such is indeed the case with the successful memory function approach in kinetic theory of classical liquids.[2]

Once the memory function $\Lambda(t)$ is determined, the linear Eq. (2) is readily solved to yield

$$x(t) = a\sum_{\mu} c_\mu \exp(\lambda_\mu t), \tag{3}$$

where c_μ are the residues at poles λ_μ of the Laplace transform $x(z)/a$, i.e.,

$$[z - \omega - \Lambda(z)]^{-1} = \sum_{\mu} c_\mu/(z - \lambda_\mu). \tag{4}$$

The solution (3) seems to indicate that its usefulness will not be limited to the decaying systems mentioned above, where all the λ_μ's have a negative real part.

In Sec. 2 we shall consider a single-variable case to illustrate the essential feature of our approach. Considerable simplification is made by introducing an assumption on the nonlinearity, and the memory function is found to be an infinite continued fraction, quite similar to that obtained by Mori in physical equilibrium systems.[3,4] When the assumption is not valid, the memory function is given by a complicated combination of infinite continued fractions. Section 3 discusses the system of several variables described by Eqs. (1a) and (1b). We introduce an expansion of an analytic function of several variables in terms of different orders at a zero, and derive a general formula for the memory function $\Lambda(t)$. Section 4 analyzes a heavily damped anharmonic oscillator as a simple illustrative example. Each successive memory function is seen to decay on a shorter time scale, and we approximate a higher-order memory function by a delta function (an instantaneous decay) to obtain a result in excellent agreement with the exact solution. The final section is devoted to some concluding remarks.

2. A SINGLE-VARIABLE CASE

Let us begin with a simple system described by a first-order ordinary differential equation

$$\dot{x}(t) = f(x(t)), \tag{5a}$$

$$x(0) = a \neq 0, \tag{5b}$$

where the function $f(x)$ is arbitrarily nonlinear in x. The initial value is assumed to be nonvanishing for the reason to be

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mentioned below.

In accordance with the theory of generalized Langevin equations,[1] we extract from the nonlinear function $f(x)$ a linear part so that the remainder is orthogonal at $t=0$ to x; i.e.,

$$f(x)=\omega x+x_1, \tag{6}$$

$$(x_1(0),x(0))=0. \tag{7}$$

The inner product is defined in Ref. 1 by the average over a statistical distribution of the initial value $x(0)$, and in the present case the distribution function is a delta function $\delta(x(0)-a)$ corresponding to the fixed initial value (5b). Thus, Eq. (7) becomes $x_1(0)a=0$, where $x_1(0)$ is a nonlinear function of a, and since $a\neq 0$, we have

$$x_1(0)=0. \tag{8}$$

This defines ω in Eq. (6) as

$$\omega=f(a)/a, \tag{9}$$

in terms of which the nonlinear part x_1 is now defined by

$$x_1=f(x)-\omega x, \tag{10}$$

and the evolution equation (5a) becomes

$$\dot{x}(t)=\omega x(t)+x_1(t). \tag{11}$$

Note that the condition (8) implies that the nonlinearity disappears in Eq. (11) at $t=0$. The initial nonlinearity is fully included in the "renormalized" frequency ω defined by Eq. (9). Note also that, if $x(0)=0$, the condition (8) implies $\dot{x}(0)=0$, which is not the case in general. This is the reason that we have assumed $x(0)\neq 0$ in Eq. (5b).[4]

The essential point of the present approach is to treat $x_1(t)$, which is a nonlinear function of $x(t)$, as a new variable, and to consider the nonlinear equation (11) for $x(t)$ as a linear equation for $x(t)$ and $x_1(t)$.

The evolution equation for the variable $x_1(t)$ is found as follows: We assume[6] for simplicity that x_1 is of first order at the zero a, i.e.,

$$x_1=(x-a)\phi_1(x), \quad \phi_1(a)\neq 0. \tag{12}$$

Then, using Eq. (11) for $\dot{x}$, we have

$$\dot{x}_1=[\phi_1(x)+(x-a)\phi_1'(x)](\omega x+x_1)=f_1(x). \tag{13}$$

As in Eq. (6) we extract from this function a linear term $\alpha_1 x$, where

$$\alpha_1=f_1(a)/a=\phi_1(a)\omega. \tag{14}$$

The remainder $\tilde{f}_1(x)=f_1(x)-\alpha_1 x$ is of first order at the zero a. Hence, we extract x_1 from $\tilde{f}_1$ so that $\tilde{f}_1=\omega_1 x_1+x_2$. If we require that ω_1 be a constant and that x_2 be of higher order at a than x_1, then ω_1 is uniquely determined by

$$\omega_1=\lim_{x\to a}[f_1(x)-\alpha_1 x]/x_1. \tag{15}$$

The proof is obvious by noting that $x_2/x_1\to 0$ as $x\to a$. The residual x_2 is also uniquely determined by

$$x_2=f_1(x)-\alpha_1 x-\omega_1 x_1. \tag{16}$$

The evolution equation (13) is now

$$\dot{x}_1(t)=\alpha_1 x(t)+\omega_1 x_1(t)+x_2(t), \tag{17}$$

which is linear in the variables x, x_1, and x_2.

We repeat this procedure. The variable x_2 is of second or higher order at a; we assume for simplicity that it is of second order, i.e.,

$$x_2=(x-a)^2\phi_2(x), \quad \phi_2(a)\neq 0. \tag{18}$$

Then, $\dot{x}_2$ is of first order and no longer contains a term linear in x; i.e., the variable x_2 is coupled only with x_1, x_2, and a new higher-order variable x_3. In general we assume that

$$x_n=(x-a)^n\phi_n(x), \quad \phi_n(a)\neq 0. \tag{19}$$

Then, since

$$\dot{x}_n=(x-a)^{n-1}[n\phi_n(x)+(x-a)\phi_n'(x)](\omega x+x_1)$$
$$=f_n(x) \tag{20}$$

is of order $n-1$, we extract as in Eqs. (14) and (15) x_{n-1} and x_n from f_n with the coefficients

$$\alpha_n=\lim_{x\to a} f_n(x)/x_{n-1}=n\omega a\phi_n(a)/\phi_{n-1}(a), \tag{21}$$

$$\omega_n=\lim_{x\to a}[f_n(x)-\alpha_n x_{n-1}]/x_n, \tag{22}$$

and define a new higher-order variable

$$x_{n+1}=f_n(x)-\alpha_n x_{n-1}-\omega_n x_n \tag{23}$$

to obtain a linear evolution equation

$$\dot{x}_n(t)=\alpha_n x_{n-1}(t)+\omega_n x_n(t)+x_{n+1}(t). \tag{24a}$$

Instead of a single nonlinear equation (5a), we now have an infinite chain of linear equations (24a) with $n=0,1,2,\ldots$, where $x_0=x$, $\alpha_0=0$, and $\omega_0=\omega$. The initial condition is

$$x(0)=a\neq 0,$$
$$x_n(0)=0, \quad n\geqslant 1. \tag{24b}$$

By virtue of the linearity, the solution to Eq. (24a) is readily obtained. In terms of the Laplace transforms $x_n(z)$, we have

$$x_n(z)=\Xi_n(z)\alpha_n x_{n-1}(z), \tag{25}$$

where

$$\Xi_n(z)=[z-\omega_n-\Xi_{n+1}(z)\alpha_{n+1}]^{-1}. \tag{26}$$

The lowest-order equation (11) then takes the form of Eq. (2) with the memory function given by $\Lambda(t)=\Xi_1(t)\alpha_1$, where $\Xi_1(t)$, normalized at $t=0$, is the inverse Laplace transform of an infinite continued fraction

$$\Xi_1(z)=\cfrac{1}{z-\omega_1-\cfrac{\alpha_2}{z-\omega_2-\ddots}}. \tag{27}$$

The nonlinear effect can thus be converted exactly into the linear memory effect, and we have now the solution (3). Our problem is therefore reduced to the calculation of $\Xi_1(z)$, which in turn is reduced to the calculation of $\Xi_2(z)$, and so on. We expect that the memory function Ξ_n becomes easily amenable to approximation with increasing order n. An example will be seen in Sec. 4.

Let us note here the formal similarity of the present results to the generalized Langevin equation.[3,1] The generalized Langevin equation reduces to the deterministic equation (2) since the random force, which is given by a linear

combination of the initial higher-order variables,[1] identically vanishes in the present case. We note also that the memory function (27) is identical in form to Mori's one.[3] Our system is, however, nonstationary and may even by nonphysical, while Mori has discussed physical equilibrium systems. The similarity of the memory function is therefore accidental and due entirely to the simplifying assumption (19). When this assumption does not hold, the variable x_n is coupled not only with x_{n-1}, x_n, and x_{n+1}, but also with $x_{n-2},...,x_1$, and x, as will be seen in the next section. The simple memory function (27) then becomes a complicated combination of infinite continued fractions. Including such a single-variable system as a special case, we now proceed to a several-variable case to find a general formula of the memory function.

3. SEVERAL-VARIABLE CASE

One of the key points of the preceding section is to decompose nonlinear functions into several terms of different orders at a zero; see Eq. (24a). To extend this formalism to the system of several variables described by Eqs. (1a) and (1b), we need some theorems on functions of several variables.

A. Decomposition into terms of different orders

We shall consider in this section complex-valued functions.

Definition 1: We say that a function $f(z)$ of n complex variables $z = (z_1,...,z_n)$, analytic in a neighborhood of a zero (let it be $z = 0$), is *of order* $\nu = (\nu_1,...,\nu_n)$ *at the zero* if f is expressed by

$$f(z) = z^{\nu}\phi(z); \quad \phi(0) \neq 0, \tag{28}$$

where $z^{\nu} = z_1^{\nu_1}...z_n^{\nu_n}$, ν_i are nonnegative integers, not all zero, and ϕ is analytic in a neighborhood of $z = 0$.

Contrary to the single-variable case, an analytic function $f(z)$ does not necessarily take the form (28), even if it has a zero at $z = 0$. Our task is now to decompose a given function into terms of different orders.

Theorem 1: Given an order $\nu = (\nu_1,...,\nu_n)$, then for every function $f(z)$ analytic in a neighborhood of the origin there exist functions $g(z)$ and $h(z)$ both analytic in a neighborhood of the origin such that

$$f(z) = z^{\nu}g(z) + h(z). \tag{29}$$

The functions $g(z)$ and $h(z)$ are uniquely determined by Eq. (29) together with the requirement that h consist of terms containing a lower power than those in z^{ν} in at least one of the variables $z_1,...,z_n$.

Proof: We repeatedly apply Späth's theorem.[7] First, we divide f by $z_1^{\nu_1}$ to obtain

$$f(z) = z_1^{\nu_1}g_1(z) + \sum_{k=0}^{\nu_1-1} h_{1k}(z_2,...,z_n)z_1^k,$$

where g_1 and h_{1k} are analytic in a neighborhood of the origin. Next, we divide g_1 by $z_2^{\nu_2}$ to define analytic functions $g_2(z)$ and $h_{2k}(z_1,z_3,...,z_n)$, $0 \leqslant k \leqslant \nu_2 - 1$; i.e., in general

$$g_{i-1}(z) = z_i^{\nu_i}g_i(z) + \sum_{k=0}^{\nu_i-1} h_{ik}(z_1,...,z_{i-1},z_{i+1},...,z_n)z_i^k$$

for $i = 2,...,n$, where g_i and h_{ik} are all analytic in a neighborhood of the origin. Equation (29) then follows with

$$g(z) = g_n(z), \tag{30}$$

$$h(z) = \sum_{i=1}^{n} z_1^{\nu_1}...z_{i-1}^{\nu_{i-1}} \times \sum_{k=0}^{\nu_i-1} h_{ik}(z_1,...,z_{i-1},z_{i+1},...,z_n)z_i^k, \tag{31}$$

where $z_1^{\nu_1}...z_{i-1}^{\nu_{i-1}} = 1$ for $i = 1$. It is obvious that g and h are analytic in a neighborhood of the origin. The uniqueness of g and h follows from the uniqueness of the power series expansion of $f(z)$ and from the fact that no term in h contains z^{ν}.

Remark: If $g(0) = D^{\nu}f(0)/\nu! \neq 0$, we may call $z^{\nu}g(z)$ the νth-order component of f.

Corollary: Let a function $f(z)$ analytic in a neighborhood of a zero, $z = 0$, be given. Let all the orders $\nu_i = (\nu_1^i,...,\nu_n^i)$ be arranged in a certain sequence $\nu_1,\nu_2,\cdots$. Then, corresponding to the sequence $\{\nu_i\}$, the function $f(z)$ is decomposed into several (N) terms of different orders at the zero as follows:

$$f(z) = \sum_{i=1}^{N} z^{\mu_i}g_i(z), \quad g_i(0) \neq 0, \tag{32}$$

where $\mu_i = (\mu_1^i,...,\mu_n^i)$ are orders of which $f(z)$ has a nonvanishing component and g_i are analytic in a neighborhood of $z = 0$.

Proof: Apply Theorem 1 with $\nu = \nu_1$, then with $\nu = \nu_2$, and so on. If the first nonvanishing component is of order $\nu_j = \mu_1$, then we have $f(z) = z^{\mu_1}g_1(z) + h_1(z)$ with $g_1(0) \neq 0$, where g_1 and h_1 are analytic in a neighborhood of the origin. We further apply Theorem 1 to the function $h_1(z)$ with $\nu = \nu_{j+1}, \nu_{j+2},\cdots$. Denoting the number of nonvanishing components by N (which may possibly be infinite), we obtain Eq. (32).

Remark: An example of the sequence of the orders is $\nu_1 = (1,0,...,0)$, $\nu_2 = (0,1,0,...,0),...$, or, in terms of z^{ν_i},

$$z_1,...,z_n,z_1^2,...,z_1z_n,z_2^2,...,z_2z_n,...,z_n^2,z_1^3,\cdots. \tag{33}$$

If, instead, a "higher"-order ν_i precedes a "lower" one $\nu_{i'}$, i.e., $\nu_k^i \geqslant \nu_k^{i'}, 1 \leqslant k \leqslant n$, for some $i < i'$, then a term of higher-order ν_i is separated from that of lower-order $\nu_{i'}$ in the decomposition (32), and thus N increases.

Theorem 2: Given L functions, of different orders at a zero, $z = 0$,

$$u_l(z) = z^{\nu_l}\phi_l(z), \quad \phi_l(0) \neq 0, \quad 1 \leqslant l \leqslant L, \tag{34}$$

then for every function $f(z)$ analytic in a neighborhood of the origin there exist L constants c_l and a function $g(z)$ analytic in a neighborhood of the origin such that

$$f(z) = \sum_{l=1}^{L} c_l u_l(z) + g(z). \tag{35}$$

If we require that $D^{\nu_l}g(0) = 0$ for every l, i.e., if $g(z)$ has no term of the same powers as ν_l, then the constants c_l, then the constants c_l, and hence the function g, are uniquely determined.

Proof: Expand both sides of Eq. (35) in powers of $z = (z_1,...,z_n)$. We assume without any loss of generality that

the L functions u_l have been numbered such that the power series expansion of u_l does not contain terms proportional to $z^{\nu_{l'}}$, $1 \leqslant l' \leqslant l-1$; i.e., $D^{\nu_{l'}} u_l(0) = 0$. Then

$$u_l(z) = z^{\nu_l}\phi_l(0) + \sum_{l'=l+1}^{L} a_{ll'} z^{\nu_{l'}} + g_l(z), \tag{36}$$

where $D^{\nu_{l'}} g_l(0) = 0$, $1 \leqslant l' \leqslant L$. Also,

$$f(z) = \sum_{l=1}^{L} f_l z^{\nu_l} + \tilde{g}(z) \tag{37}$$

with $D^{\nu_l}\tilde{g}(0) = 0$, $1 \leqslant l \leqslant L$. Denoting that $\mathbf{u} = (u_1 \cdots u_L)^T$, $\mathbf{z} = (z^{\nu_1} \cdots z^{\nu_L})^T$, $\mathbf{g} = (g_1 \cdots g_L)^T$, $\mathbf{f} = (f_1 \cdots f_L)^T$, $\mathbf{c} = (c_1 \cdots c_L)^T$, and

$$A = \begin{pmatrix} \phi_1(0) & a_{12} & a_{13} & \cdots & a_{1L} \\ & \phi_2(0) & a_{23} & \cdots & a_{2L} \\ 0 & & & & \phi_L(0) \end{pmatrix}, \tag{38}$$

where the superscript T implies transposition, we rewrite Eq. (35) as

$$\mathbf{f}^T\mathbf{z} + \tilde{g} = \mathbf{c}^T A\mathbf{z} + \mathbf{c}^T\mathbf{g} + g.$$

Since the monomials z^{ν_l} are linearly independent, we have $\mathbf{f}^T = \mathbf{c}^T A$, and since A is nonsingular, we have a unique solution

$$\mathbf{c}^T = \mathbf{f}^T A^{-1}. \tag{39}$$

Remark: The functions u_l are linearly independent of each other, as is easily verified. We shall call $c_l u_l$ the u_l component of f.

Theorem 3: Given L functions (34) and a sequence of all the orders, $\nu_1, \nu_2, \ldots$, then for every function $f(z)$ analytic in a neighborhood of a zero, $z = 0$, there exist L unique constants c_l and functions $u_{L+1}(z), \ldots, u_N(z)$ such that

$$f(z) = \sum_{l=1}^{L} c_l u_l(z) + \sum_{l=L+1}^{N} u_l(z), \tag{40}$$

where all the terms are of different orders at the zero.

Proof: Apply Theorem 2 to determine the constants c_l and a residual $g(z)$. Then apply Corollary to Theorem 1 to the function $g(z)$ to find $u_l, L+1 \leqslant l \leqslant N$.

Remark: We have in mind the case that the expansion (40) terminates at a relatively small N. Then the expansion is useful for practical purpose in contrast to, e.g., the Taylor series expansion, in which an infinite number of terms may arise.

B. Nonlinear system of several variables

Let us now turn to the system described by Eqs. (1a) and (1b), and express the nonlinear effect and the effect of coupling with the irrelevant variables $\mathbf{y} = (y_1 \cdots y_n)^T$ as a linear memory effect.

As before we extract from $f(x,\mathbf{y})$ a linear term ωx such that the residual $f - \omega x$ vanishes at $t = 0$; i.e.,

$$\omega = f(a,\mathbf{b})/a, \tag{41}$$

where $\mathbf{b} = (b_1 \ldots b_n)^T$. Since the function $f - \omega x$ vanishes at $X = x - a = 0$ and $\mathbf{Y} = \mathbf{y} - \mathbf{b} = 0$, we apply the Corollary to Theorem 1 to decompose it into several (N_1) terms of different orders at the zero, $(X,\mathbf{Y}) = 0$. Thus,

$$f(x,\mathbf{y}) - \omega x = \sum_{i=1}^{N_1} \beta_i x_{1i}, \tag{42}$$

$$x_{1i} = X^{\nu_{1i}}\mathbf{Y}^{\mu_{1i}}\phi_{1i}(X,\mathbf{Y}), \quad \phi_{1i}(0,0) \neq 0, \tag{43}$$

where $\mu_{1i} = (\mu_1^{1i}, \ldots, \mu_n^{1i})$ and $\mathbf{Y}^{\mu}$ stands for $Y_1^{\mu_1} \cdots Y_n^{\mu_n}$. In Eq. (42) we have introduced numerical factors β_i for convenience, although they can be included in ϕ_{1i}. Our first equation is now

$$\dot{x}(t) = \omega x(t) + \sum_{i=1}^{N_1} \beta_i x_{1i}(t), \tag{44}$$

which we regard as a linear equation for $x, x_{11}, \ldots, x_{1N_1}$, not a nonlinear equation for x and $\mathbf{y}$.

Let us construct evolution equations for $\mathbf{x}_1 = (x_{11} \cdots x_{1N_1})^T$. We obtain from Eqs. (43) and (1a)

$$\dot{\mathbf{x}}_1(t) = \mathbf{f}_1(x(t),\mathbf{y}(t)) \tag{45}$$

and extract from $\mathbf{f}_1$ a linear term $\alpha_1 x$; the coefficient is defined as in Eq. (41) by

$$\alpha_1 = \mathbf{f}_1(a,\mathbf{b})/a \tag{46}$$

so that the remaining term denoted by $\tilde{\mathbf{f}}_1(x,\mathbf{y}) = \mathbf{f}_1(x,\mathbf{y}) - \alpha_1 x$ vanishes at $x = a$ and $\mathbf{y} = \mathbf{b}$. We then apply Theorem 3 to each element of $\tilde{\mathbf{f}}_1$ to extract the x_{11}-, ...,. and x_{1N_1}-components and to define N_2 new variables $\mathbf{x}_2 = (x_{21} \cdots x_{2N_2})^T$,

$$x_{2j} = X^{\nu_{2j}}\mathbf{Y}^{\mu_{2j}}\phi_{2j}(X,\mathbf{Y}),$$
$$\phi_{2j}(0,0) \neq 0, \quad 1 \leqslant j \leqslant N_2 \tag{47}$$

such that

$$\dot{\mathbf{x}}_1(t) = \alpha_1 x(t) + \Omega_1 \mathbf{x}_1(t) + B_1 \mathbf{x}_2(t). \tag{48}$$

Here Ω_1 is an $N_1 \times N_1$ matrix whose ith row is

$$(\omega_1^{1i} \cdots \omega_{N_1}^{1i}) = (f_{11}^{1i} \cdots f_{1N_1}^{1i}) \times \begin{pmatrix} \phi_{11}(0) & a_{12}^1 & a_{13}^1 & \cdots & a_{1N_1}^1 \\ & \phi_{12}(0) & a_{23}^1 & \cdots & a_{2N_1}^1 \\ & & & \cdots & \\ 0 & & & & \phi_{1N_1}(0) \end{pmatrix}^{-1}, \tag{49}$$

where $f_{1i'}^{1i}$ is the coefficient of $X^{\nu_{1i'}}\mathbf{Y}^{\mu_{1i'}}$ in the expansion of the ith element of $\tilde{\mathbf{f}}_1$, and $a_{ii'}^1$ is that in the expansion of x_{1i}. The $N_1 \times N_2$ matrix $B_1 = (\beta_j^{1i})$ consists of numerical factors β_j^{1i} involved in the x_{2j}-term in the ith element of $\tilde{\mathbf{f}}_1$. If two elements of $\tilde{\mathbf{f}}_1$ have a same order term of the form (47) with different ϕ_{2j}, then we define x_{2j} by one of them and apply Theorem 3 to the other to extract the x_{2j}- and other components.

Continuing in this way, we introduce a sequence of variables $\mathbf{x}_n = (x_{n1} \ldots x_{nN_n})^T, n = 1,2,\ldots$, and construct evolution equations for them. The difference from the simple case of Sec. 2 is that, besides the multidimensionality, there is no reason that the variable $\mathbf{x}_n$ is coupled only with $\mathbf{x}_{n-1}, \mathbf{x}_n$, and $\mathbf{x}_{n+1}$. We therefore write

$$\dot{\mathbf{x}}_n(t) = \sum_{m=0}^{n-1} A_{nm}\mathbf{x}_m(t) + \Omega_n \mathbf{x}_n(t) + B_n \mathbf{x}_{n+1}(t),$$
$$n = 0,1,2,\ldots, \tag{50a}$$

where, for $n=0$, $x_0=x$, $A_{0m}=0$, $\Omega_0=\omega$, and $B_0=(\beta_1...\beta_{N_1})$. The $N_n\times 1$ matrix A_{n0} is defined by $A_{n0}=\dot{\mathbf{x}}_n(0)/a=\alpha_n$, and the $N_n\times N_m$ matrix $A_{nm}=(\alpha_{mj}^{ni})$ and the square matrix $\Omega_n=(\omega_i^{ni})$ are determined by applying Theorem 3 to $\dot{x}_{ni}-\alpha_{ni}x$ with $\{u_1,...,u_L\}=\{x_{11},...,x_{1N_1},...,x_{n1},...,x_{nN_n}\}$. The matrix $B_n=(\beta_k^{ni})$ consists of extra numerical factors of new variables $x_{n+1k}, 1\leqslant k\leqslant N_{n+1}$. Instead of the original equations (1a) and the initial condition (1b) we now have the infinite set of coupled linear Eqs. (50a), which are subject to the initial condition

$$x(0)=a\neq 0,$$
$$\mathbf{x}_n(0)=0, \quad n\geqslant 1. \tag{50b}$$

A closed equation for $x(t)$ can be derived by eliminating the variables $\mathbf{x}_1,\mathbf{x}_2,...$ from the coupled equations (50a). The Laplace transform in time leads to

$$\mathbf{x}_n(z)=\sum_{m=0}^{n-1}\Lambda_{nm}(z)\mathbf{x}_m(z), \tag{51}$$

$$\Lambda_{nm}(z)=[zI-\Omega_n-B_n\Lambda_{n+1n}(z)]^{-1}\times[A_{nm}+B_n\Lambda_{n+1m}(z)], \tag{52}$$

where I is an identity matrix. Combining this result for $n=1$ with the first equation in Eqs. (50a), we arrive at Eq. (2) with the memory function given by

$$\Lambda(t)=\sum_{i=1}^{N_1}\beta_i\Lambda_i(t), \tag{53}$$

where $\Lambda_i(t)$ is the ith element of the $N_1\times 1$ matrix $\Lambda_{10}(t)$. The Laplace-transformed memory function is therefore given by the following complicated combination of infinite continued fractions:

$$\Lambda_{10}(z)=\Xi_1(z)\{A_{10}+B_1\Xi_2(z)[A_{20}+B_2\Xi_3(z)(A_{30}+...)]\},$$
$$\Xi_n(z)=[zI-\Omega_n-B_n\Lambda_{n+1n}(z)]^{-1}. \tag{54}$$

4. A SIMPLE EXAMPLE

Before applying the general formula (54) of the memory function to practical problems, let us apply the results of Sec. 2 to a simple illustrative example to see the effectiveness of our approach. Consider a damped anharmonic oscillator described by $m\ddot{q}+\gamma\dot{q}=-[kq+bq^3]$, $q(0)=q_0\neq 0$, where q is the coordinate, m the mass, γ the damping constant, and the right-hand side represents a restoring force. For simplicity we confine ourselves to a heavily damped case, where the $m\ddot{q}$ term can be discarded.[8] We then have

$$dx/d\tau=-[x+\beta x^3], \tag{55a}$$
$$x(0)=1 \tag{55b}$$

in terms of dimensionless quantities

$$x=q/q_0, \quad \tau=(k/\gamma)t, \quad \beta=bq_0^2/k. \tag{56}$$

Starting with $f_0(x)=-(x+\beta x^3)$, we repeat the calculation from Eq. (20) to Eq. (24a). The higher-order variables

$$x_n=(2n-1)\beta(1-x^2)x_{n-1} \tag{57}$$

satisfy the assumption (19), and the results of Sec. 2 can apply. The memory function is given by Eq. (27), where

$$\omega_n=-(4n+1)\beta-(2n+1),$$
$$\alpha_n=2n(2n-1)\beta(1+\beta). \tag{58}$$

In the present dissipative system we expect that a higher-order memory function decays on a shorter time scale than those of the lower-order ones. In fact, it is seen from Eqs. (26) and (58) that $\dot{\Xi}_n(\tau)=-|\omega_n|\Xi_n(\tau)+\cdots$ and $|\omega_N|<|\omega_{n+1}|$ for $\beta>-0.5$. Let us therefore approximate[3]

$$\Xi_{n+1}(t)\simeq\xi\delta(\tau). \tag{59}$$

It then follows from Eq. (26) that

$$\Xi_m(z)=\cfrac{1}{z-\omega_m-\cfrac{\alpha_{m+1}}{z-\omega_{m+1}-\ddots-\cfrac{\alpha_n}{z-\omega_n-\xi\alpha_{n+1}}}} \tag{60}$$

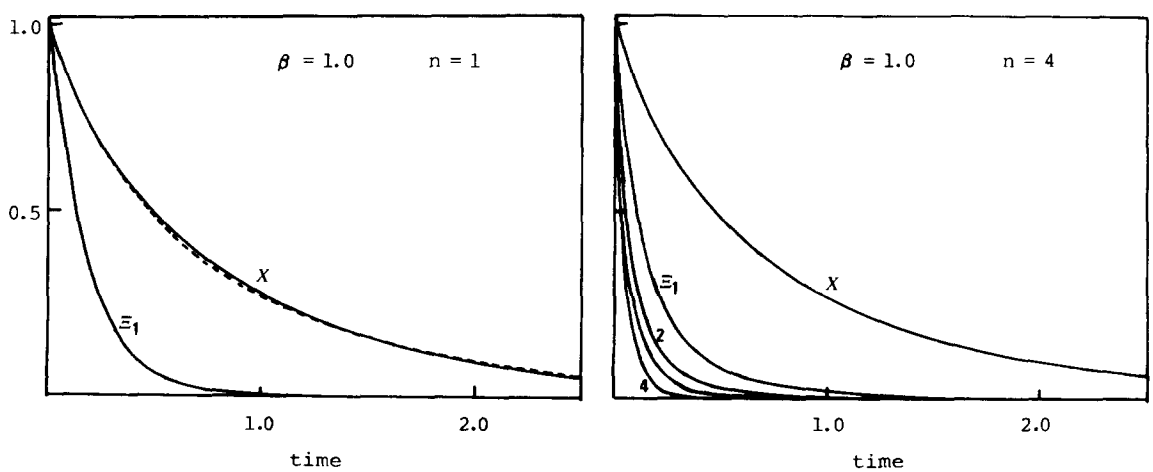

FIG. 1. Solution $x(\tau)$ and memory functions $\Xi_m(\tau)$ for a heavily damped cubic anharmonic oscillator at $\beta=1.0$ in the approximation (59) with $n=1$ and 4. The dotted line represents the exact solution (63). The numerals refer to the order m of the memory functions $\Xi_m(\tau)$.

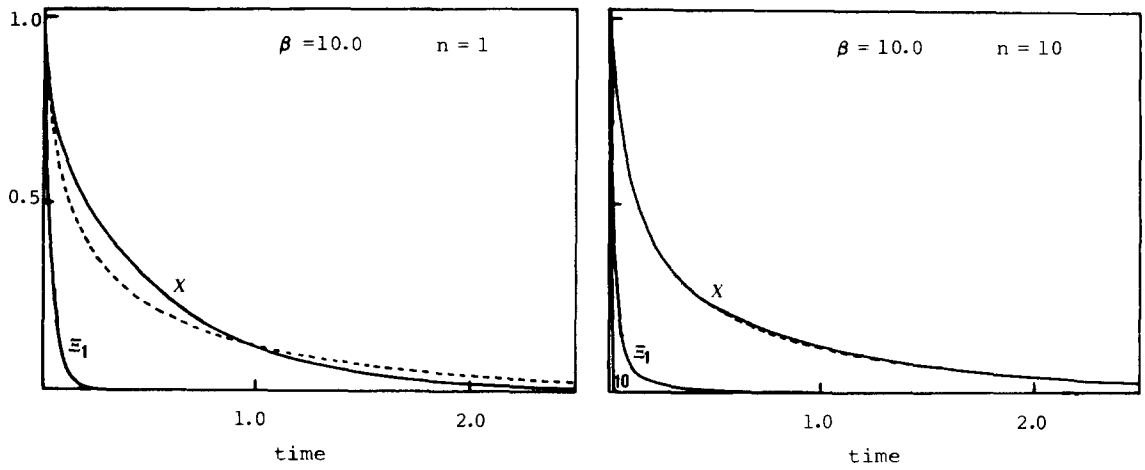

FIG. 2. Same as for Fig. 1 except that $\beta = 10.0$ (a strongly nonlinear case).

for $m = 1,2,...,n$, in terms of which we have the solution

$$x(z) = \frac{1}{z - \omega - \Xi_1(z)\alpha_1}. \tag{61}$$

We determine the unknown parameter ξ so that the solution (61) gives the correct value of the relaxation time defined by

$$\tau_0 = x(z = 0) = \int_0^\infty x(\tau)d\tau, \tag{62}$$

which is assumed to be given.

The exact solution to Eqs. (55a) and (55b), on the other hand, is

$$x(\tau) = [(1 + \beta)e^{2\tau} - \beta]^{-1/2}. \tag{63}$$

The relaxation time is given by

$$\tau_0 = \begin{cases} \beta^{-1/2}\arcsin[\beta/(1+\beta)]^{1/2}, & \beta \geqslant 0, \\ (-\beta)^{-1/2}\ln\{[1+(-\beta)^{1/2}]/(1+\beta)^{1/2}\}, & -1 \leqslant \beta \leqslant 0. \end{cases} \tag{64}$$

For $\beta < -1$, $x(\tau)$ increases with time, and the relaxation time (62) is meaningless.

We have made numerical calculations of $x(\tau)$, as well as the sequence of the memory functions, in the approximation (59), and compared the result with the exact solution (63). In the present approximation the memory function $\Xi_{n+1}(\tau)$ is the delta function, $\Xi_n(\tau)$ is a single exponential, $\Xi_m(\tau)$, $m = n-1,...,1$, are a sum of $n - m + 1$ exponentials, and $x(\tau)$ consists of $n + 1$ exponentials. For $|\beta| \ll 1$ the nonlinear effect is unimportant; we are not concerned with this trivial case. The result for $\beta = 1.0$ is shown in Fig. 1. A remarkably good agreement of our solution with the exact one is seen even in a simple approximation (59) with $n = 1$. They become indistinguishable in the figure at $n = 4$. For a strongly nonlinear case of $\beta = 10.0$, the agreement is worse (Fig. 2); however, a close agreement is obtained by taking account of ten memory functions [and the eleventh one $\Xi_{11}(\tau) \propto \delta(\tau)$ not plotted in the figure]. When β is negative, oscillatory memory functions appear corresponding to complex poles of $\Xi_m(z)$. Figure 3 shows the results at $\beta = -0.5$; again, an excellent agreement is seen at $n = 8$.

Figures 1–3 show that a higher-order memory function decays more rapidly than the lower-order ones. The memory function approach is obviously useful in this case. The usefulness will, however, not be restricted to such a case, as mentioned in the Introduction. Indeed, for $-10 \leqslant \beta < -1$, where $x(\tau)$ and the memory functions are not bounded, we have made a preliminary calculation by simply putting $\Xi_{n+1} \simeq 0$ and obtained reasonably good results.

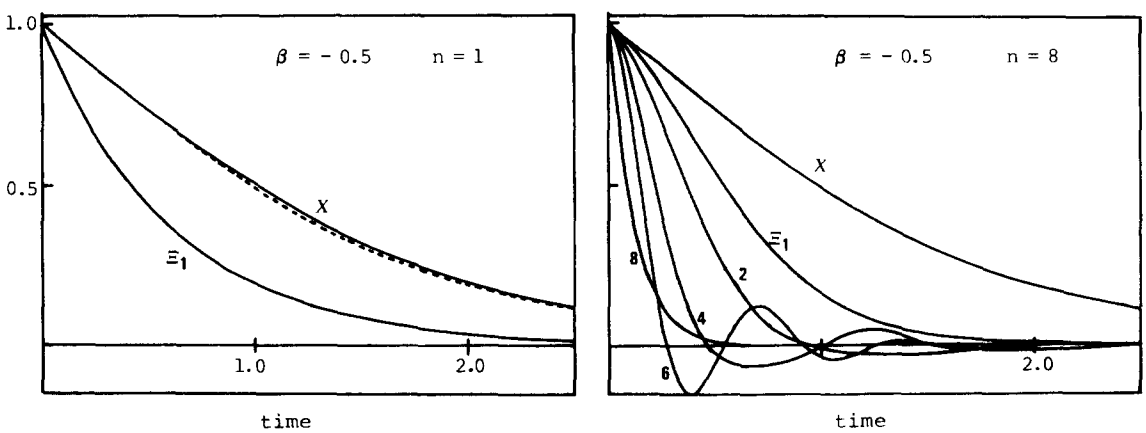

FIG. 3. Same as for Fig. 1 except that $\beta = -0.5$. Oscillatory memory functions appear for $\beta < 0$.

5. CONCLUDING REMARKS

The exact linear Eq. (2) does not imply that the linear superposition law can apply to the nonlinear problems. When $x_a(t)$ and $x_b(t)$ are solutions to the linear Eq. (2) with given ω and $\Lambda(t)$, a sum $x_a(t)+x_b(t)$ is of course a solution to Eq. (2) with the same ω and $\Lambda(t)$. However, the parameter ω and those in $\Lambda(t)$ depend on the initial values (1b), and hence, even if $x_a(t)$ is the solution to Eqs. (1a) and (1b), $x_b(t)$ and $x_a(t)+x_b(t)$ are not.

There exist several theories in which exact linear equations are constructed. An example is the Mori formalism for linear generalized Langevin equation.[3] We have also a well-known example in the quantum-statistical theory, where nonlinear equations of motion are cast into an infinite hierarchy of linear inhomogeneous equations for two-time Green's functions.[9] In contrast to the higher-order Green's functions, our "higher-order" variables $\mathbf{x}_n$ are coupled with the lower-order ones. This makes it possible to express $\mathbf{x}_n$ exactly in terms of the lower-order variables as in Eq. (51), and to obtain the closed equation (2). Another example, which is more closely related to the present approach, is that based on the Carleman linearization procedure,[10] in which a finite set of nonlinear rate equations is converted into an infinite set of linear equations.[11,12] In this approach, too, a variable is not coupled with the lower-order ones, i.e., the lower-order components are not extracted from higher-order variables. Hence, the higher-order variables will be sensitive to approximation.

The results derived in Sec. 3 for general nonlinear systems are rather complicated, and it will become increasingly difficult to calculate higher-order variables. Many of the nonlinear systems are, however, quadratic[12–15]; in this case we can find simple formulas and recursion relations, which enable us to make any higher-order calculation. Such a study is now in progress.

It should be noted that Eq. (1a) describes also the following cases:

1. When a system is described by a second-order differential equation, we take the derivative $\dot{x}$ as y_1 to obtain the first-order equations (1a).

2. For a spatially inhomogeneous case, we take spatial derivatives of x as variables $y_{n+1},\cdots$. The parameters A_{nm}, Ω_n, and B_n then depend on the spatial coordinates.

3. When evolution equations depend explicitly on t, we put $y_n(t)=t$ in Eq. (1a).[5]

Thus the present formalism is applicable to a variety of nonlinear problems such as the Van der Pol equation,[5] the Lotka–Volterra model,[13] nonlinear interaction of plasma waves,[14] nonlinear kinetics in phosphorescence decay,[15] etc. We hope to discuss in later papers the usefulness of the present approach in these practical problems.

ACKNOWLEDGMENTS

The author is much indebted to Professor H. Morinaka of Mathematics Department of Osaka Institute of Technology for discussions on the proof of our theorems. Thanks are also due to H. Tanaka for his helpful contribution to numerical calculations.

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On the gravitational phase transition in the Thomas–Fermi model

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(Received 9 December 1980; accepted for publication 13 February 1981)

The first order phase transition in an infinite system of gravitating fermions is analyzed in the canonical ensemble. Except for the question of nonmonotonicity of the mass distribution as a function of the chemical potential, we give an analytical proof for the existence of the phase transition. A single phase region is shown to exist for temperatures high compared to the gravitational energy.

PACS numbers: 05.30.Fk, 05.70.Fh, 31.20.Lr

I. INTRODUCTION

Due to negative specific heat, instabilities occur in classical models for particles interacting mutually with gravitational forces (see, e.g., Ref. 1). In the presence of a heat bath, in the canonical ensemble, the instabilities will be bridged by a phase transition.[1,2] Thirring[2] noticed that it will be the negative specific heat region which is replaced by the phase transition in a suitably truncated classical model. For fermions, due to the Pauli principle, a modification of the gravitational potential is not necessary. The analysis can start from the first principles of Newton's theory of gravitation and from quantum mechanics. From this basis some results have been obtained with complete mathematical rigor. For example, Hertel and Thirring[3] proved the exact validity of the Thomas–Fermi equation for the canonical ensemble in an appropriate thermodynamic limit. The existence of a gravitational phase transition is, however, not established with similar mathematical rigor, i.e., by a completely analytical proof. The existence of the phase transition is known from detailed numerical studies of the Thomas–Fermi equation.[4] Also in this paper we have not succeeded in giving an entirely analytical proof for the existence of a first order phase transition in the gravitating fermion model. At one point in the chain of arguments we use the nonmonotonicity of the mass distribution as a function of the chemical potential. This has been demonstrated only numerically but in a very painstaking and reliable analysis by Hertel.

Gravitating fermions are a model for a quantum continuous system, described formally for a finite particle number by the Hamiltonian

$$H_N = \sum_{i=1}^{N} \frac{-\Delta_i}{2M} - \sum_{1\le i<j\le N} \frac{\kappa M^2}{|x_i - x_j|}, \tag{1.1}$$

with Dirichlet boundary conditions on the antisymmetrized subspace of $\mathscr{L}_2(\Lambda^N)$, where $\Lambda \subset \mathbb{R}^3$ denotes either a cube of length l or a ball of radius R. The infinite system is obtained by taking an appropriate scaling and letting N tend to infinity whereas Λ is kept fixed. This limit might be called the "thermodynamic Thomas–Fermi limit", because one of the first rigorous results on the gravitating fermion model claims the existence of this limit and the exact validity of the temperature-dependent Thomas–Fermi equation for the limit system.[3]

The rigorous results about the gravitating fermion model following the quoted first achievement should be briefly mentioned: Existence of the thermodynamic Thomas–Fermi limit for the thermodynamic functions was proved for the microcanonical and canonical ensemble[5] and for the grand canonical ensemble.[6] (The ensembles are nonequivalent). The existence of the thermodynamic Thomas–Fermi limit was proved for the correlation functions[7] and for the thermodynamic states on a so-called hydro-local C^*-algebra.[8] Recently an infinite configuration space was considered,[9] and the (classical) Vlasov hydrodynamics was derived from the microscopic dynamics of a quantum mechanical model with regularized interactions.[10]

The Thomas–Fermi equation (for the canonical ensemble) is written for given (β, n, Λ) as

$$\rho(x) = \int \frac{d^3p}{(2\pi)^3} \left\{ 1 + \exp\left[\beta \left(\frac{p^2}{2M} + W(x) - \mu \right) \right] \right\}^{-1}, \tag{1.2}$$

$$W(x) = -\kappa M^2 \int_\Lambda \frac{\rho(y)}{|x-y|} d^3y, \tag{1.3}$$

$$\int_\Lambda \rho(x)\, d^3x = n, \tag{1.4}$$

with the additional important requirement that the solutions of the self-consistency equations [(1.2),(1.3),(1.4)] have to minimize the free energy functional.

We study here the existence and uniqueness of solutions of the Thomas–Fermi equation, and we shall prove—with the help of the above-mentioned numerical result, but otherwise analytically—the existence of at least two solutions, both minimizing the free energy functional. In addition, we give a high temperature domain of the thermodynamic parameters, where uniqueness of the solutions holds.

II. THOMAS–FERMI THEORY FOR GRAVITATING FERMIONS

In what follows we presuppose the canonical ensemble and spherical symmetric boundary conditions, i.e., $\Lambda \subset \mathbb{R}^3$ is a ball of radius R centered at the origin.

Definition 2.1: Given the inverse temperature $\beta > 0$, the radius R, and $n > 0$. For $y \in \mathbb{R}$ let

$$g(\beta, y) = \int \frac{d^3p}{(2\pi)^3} (1 + e^{\beta(p^2 + y)})^{-1}. \tag{2.1}$$

For gravitating fermions the potential generated by the mass distribution $\rho \in \Omega$ with the positive cone $\Omega = \{\rho \in \mathscr{L}_1(\Lambda),$

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$\rho \geqslant 0\}$ is

$$W[\rho](x) = -\int_\Lambda \rho(y)\,|x-y|^{-1}\,d^3y. \tag{2.2}$$

The Thomas–Fermi functional on Ω is given by the two conditions

$$T[\rho](x) = g(\beta, W[\rho](x) - \bar{\mu}[\rho]), \tag{2.3}$$

$$\int_\Lambda T[\rho](x)\,d^3x = n. \tag{2.4}$$

The following self-consistency equation is called the *n-equation*:

$$\rho(x) = T[\rho](x) \quad \text{for } \rho \in \Omega. \tag{2.5}$$

Possible solutions in Ω are always uniquely continued to $\mathbb{R}^3$ by

$$\rho(x) = 0 \quad \text{for } x \notin \Lambda. \tag{2.6}$$

Remark 2.2: Equation (2.3) gives $T[\rho]$ in terms of the functional $\bar{\mu}[\rho]$. Since $g(\beta,\cdot)$ is monotonic and continuous the functional $\bar{\mu}[\rho]$ is uniquely determined by condition (2.4) for each $\rho \in \Omega$. Thus, for given $\rho \in \Omega$, T is a uniquely determined functional.

Remark 2.3: We have used the following units: Fermion mass $M = \frac{1}{2}$, gravitational constant $\kappa = 4$, and $\hbar = 1$. For convenience the spin s of the fermions is set equal to zero because it shows up only in a trivial factor $2s+1$. This is no unphysical convention in nonrelativistic quantum statistics.

Definition 2.4: Given $\beta > 0$, $R > 0$, and $\mu \in \mathbb{R}$, the following self-consistency equation is called the *μ-equation*:

$$\rho(x) = T_\mu[\rho](x) = g(\beta, W[\rho](x) - \mu) \quad \text{for } \rho \in \Omega. \tag{2.7}$$

Definition 2.5: Given $\beta > 0$, $R > 0$, and $\lambda \in \mathbb{R}$, the following self-consistency equation is called the *λ-equation*:

$$\rho(x) = G_\lambda[\rho](x) = g(\beta, w[\rho](x) + \lambda) \tag{2.8}$$

with $\rho \in \bar{\Omega} = \Omega \cap \mathscr{L}_1(\Lambda, |x|^{-1}\,d^3x)$ and

$$w[\rho](x) = W[\rho](x) - W[\rho](0). \tag{2.9}$$

Remark 2.6: The *n-equation* can be also equivalently defined by the following two conditions: Given $\beta > 0$, $R > 0$, and $n > 0$, then for $\rho \in \bar{\Omega}$:

$$\rho(x) = G[\rho](x) = g(\beta, w[\rho](x) + \bar{\lambda}[\rho]), \tag{2.10}$$

$$\int_\Lambda G[\rho](x)\,d^3x = n. \tag{2.11}$$

Again $\bar{\lambda}[\rho]$ is uniquely determined by (2.11).

Definition 2.7: ρ° is a solution of the (temperature-dependent) *Thomas–Fermi equation* if and only if

(i) ρ° is solution of the n-equation,

(ii) $\Phi = \inf_{\rho \in \Omega} F_\rho[\rho] = F_\rho[\rho^\circ]$.

The *free energy functional* is

$$F_\rho[\rho] = -u[\rho] + n\bar{\mu}[\rho] - \beta^{-1}\int_\Lambda d^3x \int [d^3p/(2\pi)^3] \times \ln(1 + e^{-\beta(p^2 + W[\rho](x) - \bar{\mu}[\rho])}) \tag{2.12}$$

with

$$u[\rho] = \tfrac{1}{2}\int_\Lambda d^3x\,\rho(x) W[\rho](x). \tag{2.13}$$

$F_\rho[\cdot]$ is bounded from below on all of Ω.

Definition 2.8: If $f: \Lambda \to \mathbb{R}$ with $f(Dx) = f(x)$ holds for all $x \in \Lambda$ and $D \in \mathrm{SO}(3)$, then we define $\tilde{f}: [0,R] \to \mathbb{R}$ by $\tilde{f}(|x|) = f(x)$.

Let $\Omega_n = \{\rho \in \Omega, \int_\Lambda \rho(x)\,d^3x = n\}$, and let for each $\beta > 0$, $R > 0$, and $n > 0$ $\Omega^{(1)}_{\beta,R,n} = \{\rho \in \Omega_n \cap \mathscr{L}_q(\Lambda)$ for $q < 2$ with

(i) $\rho(Dx) = \rho(x)$ for all $x \in \Lambda$, $D \in \mathrm{SO}(3)$,

(ii) $\|\rho\|_q \leqslant d_q(\beta,R,n) = d_q$ if $q < 2$,

(iii) $\rho(x) \leqslant \hat{g}(\beta,R,n) = \hat{g}$ for all $x \in \Lambda$,

(iv) $|\rho(x) - \rho(x')| \leqslant \hat{g}(1 - e^{-\beta c_2^2 \hat{g}|x-x'|})$ for all $x,x' \in \Lambda\}$, (2.14)

where for $q < 2$

$$d_q = \left\{\frac{11}{12\pi^2}\beta^{-3/2} + \frac{1}{4\pi^2}\beta^{-1/2}\hat{\mu}\right\}\left(\frac{4\pi}{3}\right)^{1/q} R^{3/q} + \frac{1}{4\pi^2}\beta^{-1/2} n \left(\frac{4\pi}{3-q}\right)^{1/q} R^{3/q-1} + \frac{1}{6\pi^2} \times \left\{n\left(\frac{4\pi}{3-\frac{3}{2}q}\right)^{2/3q} R^{2/q-1} + \hat{\mu}\left(\frac{4\pi}{3}\right)^{2/3q} R^{2/q}\right\}^{3/2}, \tag{2.15}$$

with $\hat{\mu} = \hat{\mu}(\beta,R,n)$ defined uniquely by

$$n/|\Lambda| = g(\beta, -(n/R + \hat{\mu})), \tag{2.16}$$

where $|\Lambda|$ is the ball volume. Furthermore,

$$\hat{g} = g(\beta, -(c_p d_q + \hat{\mu})) \tag{2.17}$$

with $p^{-1} + q^{-1} = 1$, $2 < p < 3$, $\frac{3}{2} < q < 2$, and for $p < 3$

$$c_p = \| 1/|x| \|_p = \{[4\pi/(3-p)] R^{3-p}\}^{1/p}. \tag{2.18}$$

Lemma 2.9: Given $\beta > 0$, $R > 0$, and $n > 0$, if $\rho \in \Omega_n$ is a solution of the Thomas–Fermi equation, then $\rho \in \Omega^{(1)}_{\beta,R,n}$.

Proof: (2.14) (i) is a consequence of Baumgartner's theorem.[7] (2.14) (ii) follows from inequality (25) in Ref. 7 and the fact that for negative $\bar{\mu}[\rho]$'s the estimate (2.14) (ii) holds with $\hat{\mu}$ replaced by zero in (2.15), whereas for positive $\bar{\mu}[\rho]$'s it follows from Lemma 2.11 and (2.16) that $\bar{\mu}[\rho] \leqslant \hat{\mu}$. (2.14) (iii) is an immediate consequence (Ref. 7, Eqs. (28), (29)). Finally (2.14) (iv) holds by elementary calculations. □

Remark 2.10: If $\rho \in \Omega_n$ is a solution of the n-equation for each $\beta > 0$, $R > 0$, and $n > 0$ with $\rho \in \Omega_n$, then necessarily $\rho \in \bar{\Omega}^{(1)}_{\beta,R,n}$, which is the set $\Omega^{(1)}_{\beta,R,n}$ without the spherical symmetry requirement (2.14) (i).

Lemma 2.11: Let $\rho \in \Omega_n$ with $\rho(Dx) = \rho(x)$ for all $x \in \Lambda$ and $D \in \mathrm{SO}(3)$; then

(i) $W[\rho](Dx) = W[\rho](x)$ for all $x \in \Lambda$, $D \in \mathrm{SO}(3)$,

(ii) $\tilde{W}[\rho](|x|)$ is monotonic increasing in $|x| \in (0,R)$,

(iii) $\tilde{W}[\rho](R) = -n/R$,

(iv) $T[\rho](Dx) = T[\rho](x)$, $T_\mu[\rho](Dx) = T_\mu[\rho](x)$ for all $x \in \Lambda$, $D \in \mathrm{SO}(3)$,

(v) $\tilde{T}[\rho](|x|)$ and $\tilde{T}_\mu[\rho](|x|)$ are monotonic decreasing in $|x| \in (0,R)$,

(vi) $\tilde{w}[\rho](|x|)$ is monotonic increasing in $|x| \in (0,R)$,

(vii) $G[\rho](Dx) = G[\rho](x)$, $G_\lambda[\rho](Dx) = G_\lambda[\rho](x)$ for all $x \in \Lambda$, $D \in \mathrm{SO}(3)$,

(viii) $\tilde{G}[\rho](|x|)$ and $\tilde{G}_\lambda[\rho](|x|)$ are monotonic decreasing

in $|x| \in (0,R)$.

Proof: (i) is well-known, (ii) follows from elementary calculations, (iii) is Newton's theorem, (iv) and (v) are direct consequences of (i), (ii), and the definitions of $T[\rho]$, $T_\mu[\rho]$. (vi) follows trivially from (ii). (vii) and (viii) are immediate.□

Lemma 2.12: Given $\beta > 0$ and $R > 0$:

(i) For each $n > 0$, there exists at least one solution $\rho \in \Omega_n$ of the Thomas–Fermi equation.

(ii)For each $n > 0$, there exists at least one solution $\rho \in \Omega^{(1)}_{\beta,R,n}$ of the n-equation.

(iii) For each $\lambda \in \mathbb{R}$, there exists a unique solution $\rho \in \Omega^{(2)}_{\beta,R,\lambda}$ of the λ-equation.

Proof: (i) follows from the fact that the Thomas–Fermi equation is asymptotically exact: It has been proven in Refs. 3,4, and 5 that the free energy F_N of a N-particle system of gravitating fermions has a limit Φ if F_N is properly rescaled and $N \to \infty$, i.e., the thermodynamic Thomas–Fermi limit exists. The limit point Φ is expressed by a one-particle density $\rho(x)$, which fulfills the Thomas–Fermi equation, i.e., the existence of a global minimum of the free energy functional $F_\rho[\rho]$, $\rho \in \Omega_n$ has been proven for each $n > 0$.

(ii) is a trivial consequence of (i), Definition 2.7, and Lemma 2.9.

(ii) can be proved without recourse to (i) by using the argumentation in the proof of Lemma 2.15 (ii) and the Lemma 2.16. Analogously, using the same arguments for a set of ρ's slightly different from $\Omega^{(1)}_{\beta,R,n}$ and Schauder's fix point theorem, Lemma 2.12 (ii) can be proved when the representation (2.10) and (2.11) of the n-equation is used.

In (iii) the set $\Omega^{(2)}_{\beta,R,\lambda}$ is defined by

$$\Omega^{(2)}_{\beta,R,\lambda} = \{\rho \in \Omega \text{ with}$$
(i) $\rho(Dx) = \rho(x)$ for all $x \in \Lambda$, $D \in SO(3)$,
(ii) $\rho(x) \leqslant \hat{g}_\lambda = g(\beta,\Lambda)$ for all $x \in \Lambda$,
(iii) $|\rho(x) - \rho(x')| \leqslant \hat{g}_\lambda (1 - e^{-\beta c_2^2 \hat{g}_\lambda |x - x'|})$ for all
$x,x' \in \Lambda \}$. (2.19)

Again every spherical symmetric solution $\rho \in \Omega$ of the λ-equation is necessarily element of $\Omega^{(2)}_{\beta,R,\lambda}$.

(iii) has first been proved in Ref. 4 by using the equivalence of the λ-equation to Poisson's differential equation for a potential $U(\xi)$ [denoted as $W(\xi)$ in Ref. 4], $\xi = \beta^{-1/4}|x|$ with the initial conditions $U(0) = 0$ and $U'(0) = \beta\lambda$, and then applying standard theorems for ordinary differential equations. It has been proved a second time in Ref. 11 by rewriting the λ-equation, resp. Poisson's equation, as an integral equation $\rho = K_\lambda[\rho]$ and showing that K_λ is a contraction map on a complete topological space with a suitable metric.□

The μ-equation is equivalent to Poisson's differential equation for the potential $U(\xi)$ [denoted as $W(\xi)$ in Ref. 4] –as stated in (3.2) of Ref. 4 –but as a *boundary value problem* with $U(0) = 0$ and $U'(\beta^{-1/4}R) = -\beta\mu$. Therefore, one cannot expect to obtain a simple statement on the existence or uniqueness of solutions.

Definition 2.13: For each $\beta > 0$, $R > 0$, and $k > 0$ we define

$$\Omega^{(3)}_{\beta,R,k} = \{\rho \in \Omega \text{ with}$$
(i) $\rho(Dx) = \rho(x)$ for all $x \in \Lambda$, $D \in SO(3)$,
(ii) $\rho(x) \leqslant k$ for all $x \in \Lambda$,
(iii) $|\rho(x) - \rho(x')| \leqslant k(1 - e^{-\beta c_2^2 k |x - x'|})$
for all $x,x' \in \Lambda \}$. (2.20)

Remark 2.14: $\Omega^{(3)}_{\beta,R,k}$ is nonempty.

The characteristic functions $a\chi_{[0,R]}$ are in $\Omega^{(3)}_{\beta,R,k}$ if $0 \leqslant a \leqslant k$.

Lemma 2.15: Given $\beta > 0$, $R > 0$, and $\mu \in \mathbb{R}$.

(i) If $\mu > \mu_0$, where $\mu_0 = \mu_0(\beta,R)$ is the unique solution of

$$g(\beta, -\mu_0) = \tfrac{243}{16}\pi R^{-6}(1 + e^{-\beta\mu_0})^2, \tag{2.21}$$

then there exists no solution of the μ-equation in Ω.

(ii) For every $\beta > 0$, $R > 0$, and $k > 0$ there exists a $\mu_1 = \mu_1(\beta,R,k)$ uniquely defined by

$$g(\beta, -(c_1 k + \mu_1)) = k \tag{2.22}$$

such that for each $\mu < \mu_1$ there exists at least one solution of the μ-equation in the set $\Omega^{(3)}_{\beta,R,k}$.

(iii) If $k\beta c_1 < 1$ and if (β,R,k,μ) is in the domain indicated in (ii), then there exists a unique solution of the μ-equation in $\Omega^{(3)}_{\beta,R,k}$.

Proof: (i) With Lemma 2.11 we find a lower bound

$$\begin{aligned}\beta^{3/2} g(\beta, W[\rho](x) - \mu) &\geqslant (2\pi)^{-2} \int_0^{-\beta W[\rho](x)} d\eta \sqrt{\eta}\,(1 + e^{\eta + \beta W[\rho](x) - \beta\mu})^{-1} \\ &\geqslant (6\pi^2)^{-1} (n\beta/R)^{3/2} (1 + e^{-\beta\mu})^{-1},\end{aligned} \tag{2.23}$$

with $n = \int_\Lambda \rho(x)\, d^3x < \infty$, because $\rho \in \Omega$. Assuming the existence of a solution of the μ-equation turns (2.23) in an upper bound for n:

$$n \leqslant 36\pi^4 R^3 |\Lambda|^{-2} (1 + e^{-\beta\mu})^2, \tag{2.24}$$

which contradicts the lower bound

$$n \geqslant |\Lambda|\, g(\beta, -\mu) \tag{2.25}$$

for $\mu > \mu_0$.

(ii) The set $\Omega^{(3)}_{\beta,R,k}$ endowed with the $\mathscr{L}_\infty$-topology is convex and compact: It is a set of equicontinuous functions, such that $\{\rho(x), \rho \in \Omega^{(3)}_{\beta,R,k}\}$ is compact for each $x \in \Lambda$ by the Lebesgue–Borel theorem. With the theorem of Arzela–Ascoli we conclude that $\Omega^{(3)}_{\beta,R,k}$ is precompact, but it is also $\|\cdot\|_\infty$-closed. The functional $T_\mu[\cdot]$, $\mu < \mu_1$, maps $\Omega^{(3)}_{\beta,R,k}$ into $\Omega^{(3)}_{\beta,R,k}$ and is continuous in the $\|\cdot\|_\infty$-topology. Applying the fix point theorem of Schauder and Tychonoff concludes the proof. The lemma is also valid in case Λ is an open, bounded, Lebesgue-measurable region in $\mathbb{R}^3$, and if $\Omega^{(3)}_{\beta,R,k}$ is not restricted to spherical symmetric functions.

(iii) If $k\beta c_1 < 1$, then the inequality

$$\|T_\mu[\rho_1] - T_\mu[\rho_2]\|_\infty \leqslant k(1 - e^{-\beta c_1 \|\rho_1 - \rho_2\|_\infty}) \tag{2.26}$$

for $\rho_1, \rho_2 \in \Omega^{(3)}_{\beta,R,k}$ turns $T_\mu[\cdot]: \mathscr{L}_\infty(\Lambda) \to \mathscr{L}_\infty(\Lambda)$ into a contraction map on the complete topological space $\Omega^{(3)}_{\beta,R,k}$. □

Lemma 2.16: For every $\beta > 0$, $R > 0$, $n > 0$, and $x \in \Lambda$ the functionals $W[\cdot](x)$, $\bar{\mu}[\cdot]$, and $T[\cdot](x)$ are strongly continuous on $(\Omega^{(1)}_{\beta,R,n}, \|\cdot\|_\infty)$.

Proof: For W continuity follows from the trivial inequality

$$|W[\rho_1](x) - W[\rho_2](x)| \leqslant c_1 \|\rho_1 - \rho_2\|_\infty, \tag{2.27}$$

where c_1 is given by (2.18).

Let $\rho_j \in \Omega^{(1)}_{\beta,R,n}$, $j \in \mathbb{N}$, converge strongly to ρ_0, then, because $\Omega^{(1)}_{\beta,R,n}$ is closed, $\rho_0 \in \Omega^{(1)}_{\beta,R,n}$. The possible values of the chemical potential are bounded,

$$\check{\mu} \leqslant \bar{\mu}[\rho_j] \leqslant \hat{\mu}, \tag{2.28}$$

where

$$n/|\Lambda| = g(\beta, -(c_p d_q + \check{\mu})) \tag{2.29}$$

with p and q chosen as in (2.17). Let μ_0 be any accumulation point of $\{\bar{\mu}[\rho_j], j \in \mathbb{N}\}$, and $\{\rho_{j_i}, i \in \mathbb{N}\}$ a subsequence of $\{\rho_j, j \in \mathbb{N}\}$, such that $\bar{\mu}[\rho_{j_i}]$ converges to μ_0. Since $g(\beta,\cdot)$ is continuous and $g(\beta, W[\rho_j] - \bar{\mu}[\rho_j]) \leqslant \hat{g}(\beta,R,n)$, it follows by Lebesgue's convergence theorem that

$$n = \lim_{i \to \infty} \int_\Lambda T[\rho_{j_i}](x)\, d^3x = \int_\Lambda g(\beta, W[\rho_0](x) - \mu_0)\, d^3x,$$

from which $\mu_0 = \bar{\mu}[\rho_0]$ can be inferred by monotonicity of $g(\beta,\cdot)$. Continuity of $T[\cdot](x)$ is a consequence of continuity of $g(\beta,\cdot)$, $W[\cdot](x)$, and $\bar{\mu}[\cdot]$.□

Corollary 2.17: For every $\beta > 0$, $R > 0$, and $n > 0$ the free energy functional $F_\rho[\cdot]$ attains its infimum and supremum on $\Omega^{(1)}_{\beta,R,n}$ and is strongly continuous on $(\Omega^{(1)}_{\beta,R,n}, \|\cdot\|_\infty)$.

Proof: Continuity can be immediately concluded from Lemma 2.16 and (2.12). Compactness of $\Omega^{(1)}_{\beta,R,n}$ with respect to the $\mathscr{L}_\infty$-topology concludes the proof.□

For the λ-representation of the n-equation, described in Remark 2.6, one obtains analogous results: With

$$n/|\Lambda| = g(\beta, \hat{\lambda}) \tag{2.30}$$

and

$$n/|\Lambda| = g(\beta, 2c_p d_q + \check{\lambda}), \tag{2.31}$$

where p and q are chosen as in (2.17), the numbers $\hat{\lambda} = \hat{\lambda}(\beta,R,n)$ and $\check{\lambda} = \check{\lambda}(\beta,R,n)$ are uniquely defined, and for each $\rho \in \bar{\Omega}$

$$\check{\lambda} \leqslant \bar{\lambda}[\rho] \leqslant \hat{\lambda}. \tag{2.32}$$

If $\Omega^{(4)}_{\beta,R,n}$ is defined as $\Omega^{(3)}_{\beta,R,k} \cap \Omega_n$ with k replaced by $g(\beta,\check{\lambda})$, then, for each $x \in \Lambda$, $G[\cdot](x)$ and $\bar{\lambda}[\cdot]$ are continuous functionals on $\Omega^{(4)}_{\beta,R,n}$ in the $\mathscr{L}_\infty$-topology. For each $x \in \Lambda$, $G[\cdot](x)$ leaves $\Omega^{(4)}_{\beta,R,n}$ invariant. Given $\beta > 0$, $R > 0$, and $n > 0$, if $\rho \in \Omega_n$ is a solution of the Thomas–Fermi equation, then $\rho \in \Omega^{(4)}_{\beta,R,n}$.

For each solution $\rho_n \in \bar{\Omega}$ of the n-equation there exists a unique solution $\rho_\lambda \in \bar{\Omega}$ of the λ-equation with $\rho_n = \rho_\lambda$ (and $\int_\Lambda \rho_\lambda(x)\, d^3x = n$). This holds because of Lemma 2.12(iii) and with $\lambda = \bar{\lambda}[\rho_n]$, which is a unique number.

Definition 2.18: Given $\beta > 0$, $R > 0$, and $\lambda \in \mathbb{R}$. Let ρ_λ be the (unique) solution of the λ-equation; then

$$n(\lambda) = \int_\Lambda \rho_\lambda(x)\, d^3x = \int_\Lambda g(\beta, w[\rho_\lambda](x) + \lambda)\, d^3x. \tag{2.33}$$

Remark 2.19: If the n-equation has several different solutions $\rho_{n,i} \in \bar{\Omega}$, then there exist several different $\lambda_i = \bar{\lambda}[\rho_{n,i}]$ with $n(\lambda_i) = n$, i.e., $n(\lambda)$ is a nonmonotonic function. Each $\rho_{n,i} = \rho_{\lambda_i}$.

Lemma 2.20: Given $\beta > 0$ and $R > 0$:

(i) If $\lambda_1 - \lambda_2 \geqslant c_1 g(\beta,\lambda_2)$, then $n(\lambda_1) \leqslant n(\lambda_2)$.

(ii) $n(\lambda)$ is strictly monotonic decreasing for all $\lambda > \lambda_0$ with $2\beta c_1 g(\beta,\lambda_0) = 1$.

Proof: (i) The inequality

$$w[\rho_{\lambda_1}] + \lambda_1 \geqslant w[\rho_{\lambda_2}] + \lambda_2 \tag{2.34}$$

follows from the estimate

$$w[\rho_{\lambda_1}] - w[\rho_{\lambda_2}] \geqslant -c_1 g(\beta,\lambda_2).$$

(ii) From the inequality

$$\|w[\rho_{\lambda_1}] - w[\rho_{\lambda_2}]\|_\infty \leqslant c_1 \beta g(\beta,\lambda_2)\{|\lambda_1 - \lambda_2| + \|w[\rho_{\lambda_1}] - w[\rho_{\lambda_2}]\|_\infty\} \tag{2.35}$$

follows for $c_1 \beta g(\beta,\lambda_2) < 1/2$:

$$\|w[\rho_{\lambda_1}] - w[\rho_{\lambda_2}]\| < |\lambda_1 - \lambda_2|, \tag{2.36}$$

which implies $n(\lambda_1) < n(\lambda)$ if $\lambda_1 > \lambda_2$.□

Theorem 2.21: The set

$$\mathscr{N} = \{(\beta,R,n) \in \mathbb{R}^3_+ \,/\, 2\beta c_1 g(\beta,\check{\lambda}) < 1\}$$

has the following properties:

(i) $\mathscr{N}$ is not empty.

(ii) For each element of $\mathscr{N}$ there exists the solution of the Thomas-Fermi equation and it is *unique*.

(iii) If $(\beta,R,n) \in \mathscr{N}$, then $\frac{2}{3}\beta n/R < \frac{2}{5}$.

Proof: (i) Let q and p be chosen as in (2.17), and

$$n/|\Lambda| = g(\beta, 2c_p d'_q + \lambda'), \tag{2.37}$$

with d'_q being d_q with $\hat{\mu}$ replaced by μ', and

$$n/|\Lambda| = g(\beta, -\mu'), \tag{2.38}$$

which implies $\hat{\mu} \leqslant \mu'$, $d_q \leqslant d'_q$, and $\check{\lambda} \geqslant \lambda'$. Keep β and $n|\Lambda|^{-1}$ fixed, but choose R sufficiently small; then the inequality defining $\mathscr{N}$ can be validated.

(ii) Let $\rho_{n,1}$ and $\rho_{n,2}$ be two solutions of the Thomas–Fermi equation. Then $\rho_{n,1} \in \Omega^{(4)}_{\beta,R,n}$, $\rho_{n,2} \in \Omega^{(4)}_{\beta,R,n}$. Let $(\beta,R,n) \in \mathscr{N}$. Furthermore, $\lambda_1 = \bar{\lambda}[\rho_{n,1}] \geqslant \check{\lambda}$ and $\lambda_2 = \bar{\lambda}[\rho_{n,2}] \geqslant \check{\lambda}$. According to Lemma 2.20, $n(\lambda)$ is strictly monotonic decreasing for all $\lambda \geqslant \check{\lambda}$. Thus $n = n(\lambda_i)$ has the unique solution $\lambda_1 = \lambda_2$ and consequently $\rho_{n,1} = \rho_{\lambda_1} = \rho_{\lambda_2} = \rho_{n,2}$.

(iii) This inequality, describing the high temperature domain, where the temperature is compared to the gravitational energy, is a result of

$$g(\beta,\check{\lambda}) \geqslant g(\beta, 2c_p d_q + \check{\lambda}) = n/|\Lambda|.□$$

Lemma 2.22: Let $\rho_{\lambda_1} \in \bar{\Omega}$ and $\rho_{\lambda_2} \in \bar{\Omega}$ be solutions of the λ-equation, then

(i) $\lambda_1 \neq \lambda_2$ if and only if $\rho_{\lambda_1} \neq \rho_{\lambda_2}$ and

(ii) $\lambda_1 = \lambda_2$ if and only if $\rho_{\lambda_1} = \rho_{\lambda_2}$.

Proof: Since ρ_{λ_i}, $i = 1,2$, are solutions of the λ-equation, they are elements of $\Omega^{(2)}_{\beta,R,\lambda_i}$ and continuous functions. The lemma follows from

$$\rho_{\lambda_1}(0) - \rho_{\lambda_2}(0) = (1 - e^{\beta(\lambda_1 - \lambda_2)}) C(\lambda_1,\lambda_2) \tag{2.39}$$

with

$$C(\lambda_1,\lambda_2) = \frac{1}{4\pi^2} \int_0^\infty d\epsilon \sqrt{\epsilon}\, \frac{e^{\beta(\epsilon + \lambda_2)}}{(1 + e^{\beta(\epsilon + \lambda_1)})(1 + e^{\beta(\epsilon + \lambda_2)})} \tag{2.40}$$

and $C(\lambda_1,\lambda_2) > 0$ for all $\lambda_1,\lambda_2 \in \mathbb{R}$. □

Proposition 2.23: Let ρ_λ be the (unique) solution of the

λ-equation for given $\lambda\in\mathbb{R}$, $\beta>0$, and $R>0$. Then the function $\lambda\to n(\lambda)=\int_\Lambda \rho_\lambda(x)\,d^3x$ has the following properties:

(i) $\lambda\to n(\lambda)$ is an entire real analytic function.

(ii) For each $\beta>0$, $R>0$ there exists λ_1 such that, for all $\lambda>\lambda_1$, $n(\lambda)$ is strictly monotonic decreasing.

(iii) $\lim_{\lambda\to-\infty} n(\lambda)=\infty$.

(iv) $n(\lambda)\leqslant|\Lambda|\,g(\beta,\lambda)$.

Proof: (i) The λ-equation can be equivalently written as Poisson's differential equation for a renormalized potential

$$\xi^{-1}v(\xi)=\beta\tilde{w}(\beta^{1/4}\xi) \tag{2.41}$$

in the variable $\xi=\beta^{-1/4}|x|$. Instead of λ we choose the new variable $\nu=\beta\lambda$. The λ-equation is now written, similar to Ref. 4, where $U(\xi)=v(\xi)+\nu\xi$ [denoted as $W(\xi)$ in Ref. 4] has been used, as

$$v_1'(\xi)=v_2(\xi)=F_1(\xi,v_1,v_2,\nu), \tag{2.42}$$

$$v_2'(\xi)=f(v_1,\xi,\nu)=F_2(\xi,v_1,v_2,\nu), \tag{2.43}$$

where v_i' $(i=1,2)$ denotes differentiation with respect to ξ, and

$$f(v,\xi,\nu)=(\xi/\pi)\int_0^\infty d\eta\,\sqrt{\eta}\,(1+e^{\eta+\xi^{-1}v+\nu})^{-1}. \tag{2.44}$$

With the initial conditions

$$v_1(0)=0=v_2(0) \tag{2.45}$$

this system of first order ordinary differential equations becomes equivalent to the λ-equation. It has a global unique solution.[4] This fact is also visible in the equivalent integral equation.[11] We prove first that this solution is analytic in ξ and ν. Notice that in F_1 and F_2 the v_1, v_2, ξ, and ν are independent variables. From (2.42) and (2.43) we infer that if $\xi\in(0,\tilde{R})$ and $\nu\in P_\nu\subset\mathbb{R}$ (P_ν is an open interval), then

$$v_1''>0,\quad v_1'>0,\quad v_1>0 \tag{2.46}$$

and

$$v_1''\leqslant\xi c,\quad v_1'\leqslant\tfrac{1}{2}c\xi^2,\quad v_1\leqslant\tfrac{1}{6}c\xi^3, \tag{2.47}$$

with

$$c=c(\nu)=(1/\pi)\int_0^\infty d\eta\,\sqrt{\eta}\,(1+e^{\eta+\nu})^{-1}.$$

Thus it suffices to prove analyticity on the set $I_\xi\times H_v^{(2)}\times P_\nu$ with $I_\xi=(0,\tilde{R})\subset\mathbb{R}_+$, $H_v^{(2)}=(0,\hat{v}_1)\times(0,\hat{v}_2)\subset\mathbb{R}^2_+$, $\tilde{P}_\nu=(\check{\nu},\hat{\nu})$ open in $\mathbb{R}$, containing the origin. Hereby is $\hat{v}_1=\frac{1}{6}\times c(\check{\nu})\tilde{R}^3$ and $\hat{v}_2=\frac{1}{2}c(\check{\nu})\tilde{R}^2$. Clearly F_1 and $(1+e^{\eta+\xi^{-1}v_1+\nu})^{-1}$ are analytic on $I_\xi\times H_v^{(2)}\times P_\nu$ (for fixed $\eta\in\mathbb{R}$). $f(v_1,\xi,\nu)$ is analytic on $I_\xi\times H_v^{(2)}\times P_\nu$ because $(1+e^{\eta+\xi^{-1}v_1+\nu})^{-1}$ is analytic, and there exists $\eta_0\in\mathbb{R}_+$ such that

$$\max_{\eta\in\mathbb{R}_+} e^{\eta/2}|D_\xi^n D_v^m D_\nu^l\,h(\eta,\xi,v,\nu)| = e^{\eta_0/2}|D_\xi^n D_v^m D_\nu^l h(\eta_0,\xi,v,\nu)| \tag{2.48}$$

with $h(\eta,\xi,v,\nu)=(1+e^{\eta+\xi^{-1}v+\nu})^{-1}$. D_α denotes partial differentiation with respect to the variable α. (2.48) permits the application of Lebesgue's convergence theorem in interchanging of summation (of the power series) with integration.

With the multiple index j and with $z=(\xi,v_1,v_2,\nu)$ and $f_0(z)=\pi\xi^{-1}f(z)$, we conclude

$$f_0(z)=\int_0^\infty\sqrt{\eta}\,d\eta\,\lim_{N\to\infty}\sum_j^N\frac{1}{j!}D_z^j h(\eta,z_0)(z-z_0)^j, \tag{2.49}$$

$$f_0(z)=\lim_{N\to\infty}\sum_j^N\frac{1}{j!}\left\{\int_0^\infty\sqrt{\eta}\,d\eta\,D_z^j h(\eta,z_0)\right\}(z-z_0)^j. \tag{2.50}$$

[$\lim\Sigma_j(1/j!)D_z^j h(\eta,z_0)(z-z_0)^j$ converges absolutely to $h(\eta,z)$ for every $\eta\in\mathbb{R}_+$]. In (2.50) the right-hand side converges absolutely to $f_0(z)$ because of (2.48) and

$$\int_0^\infty d\eta\,\sqrt{\eta}(1/j!)|D_z^j h(\eta,z)| \leqslant\left\{\int_0^\infty d\eta\,\sqrt{\eta}\,e^{-(\eta-\eta_0)/2}\right\}(1/j!)|D_z^j h(\eta_0,z)|. \tag{2.51}$$

Thus f and F_2 are analytic on $I_\xi\times H_v^{(2)}\times P_\nu$. To verify (2.48) we note that by induction

$$D_\xi^n D_v^m D_\nu^l h=\frac{\sum_{i+j+k\leqslant N} c_{ijk}h^{-k}(e^{\eta+\xi^{-1}v+\nu})^{i+j}}{h^{-(N+1)}} \tag{2.52}$$

with $N=2^{n+m+l}-1$. Thus $-e^{\eta/2}D_\xi^n D_v^m D_\nu^l h$ decays proportional to $e^{-(\eta/2)}$, and since $h(\eta,\xi,v,\nu)$ is analytic in $\eta\in\mathbb{R}_+$ for fixed $(\xi,v,\nu)\in I_\xi\times H_v^{(2)}\times P_\nu$, the maximum in (2.48) is attained at $\eta_0\in[0,\eta_1]$ for η_1 sufficiently large (but finite).

(2.42)–(2.45) is a system of holomorphic differential equations of first order with a unique global solution. Therefore, this solution, $v_1(\xi,\nu)$ and $v_2(\xi,\nu)$, is analytic on $I_\xi\times P_\nu$ by standard theorems. The analyticity of $n(\lambda)$ is now an immediate consequence of

$$R^2\left(\frac{d}{dr}\tilde{w}(r,\lambda)\right)_{r=R}=n(\lambda). \tag{2.53}$$

Here and in what follows we indicate the dependence of $v_i(\xi)$ $(i=1,2)$ and $\tilde{w}(r)$ $(r=|x|)$ on the parameters ν or λ by writing $v_i(\xi,\nu)$ and $\tilde{w}(r,\lambda)$ respectively.

(ii) To each $\beta>0$ and $R>0$ choose $2\beta c_1 g(\beta,\lambda_1)=1$. Then (ii) follows from Lemma 2.20 (ii).

(iii) By (iv), $n(\lambda)$ is bounded from above by $|\Lambda|\,g(\beta,\lambda)$. Suppose there exists $n_0>0$ such that $n(\lambda)\leqslant n_0$ for all $\lambda\in\mathbb{R}$. With Lemma 2.12 (ii) for each $\beta>0$ and $R>0$ and $n=2n_0$ there exists a solution ρ_0 of the n-equation such that, with $\lambda_0=\tilde{\lambda}[\rho_0]\in\mathbb{R}$, ρ_{λ_0} is a solution of the λ-equation with $n(\lambda_0)=2n_0>n_0$. Continuity of $n(\lambda)$ concludes the proof.

(iv) follows trivially from $w[\rho_\lambda]\geqslant 0$ and (2.33).□

Remark 2.23 (v): Under the conditions of Proposition 2.23 there exist a $\beta_0>0$ and a $R_0>0$ and λ_2,λ_3 $(\lambda_2<\lambda_3<\lambda_1)$ such that $n(\lambda)$ is strictly monotonic increasing for all $\lambda\in[\lambda_2,\lambda_3]$.

An analytical proof of this statement is not known up to now. We present however a convincing argument based on numerical calculations by Hertel.[11] The λ-equation can be expressed as integral equation for the renormalized potential $\tilde{w}(r,\lambda)$, $r=|x|$ [11]:

$$\tilde{w}(r,\lambda)=\int_0^r s^{-2}\,ds\int_0^s 4\pi t^2\,g(\beta,\lambda+\tilde{w}(t,\lambda))\,dt. \tag{2.54}$$

$\tilde{w}(r,\lambda)$ is analytic on $(0,L_0)\times(-\lambda_4,\lambda_4)$, where L_0, $\lambda_4>0$ are arbitrary. If $n(\lambda)$ is monotonic decreasing for each r, then

also $\tilde{w}(r,\lambda)$ is monotonic decreasing for each r, because

$$\tilde{w}(r,\lambda) = \int_0^r s^{-2} n(\lambda,s)\, ds. \tag{2.55}$$

Here with $n(\lambda,s)$ the dependence of $n(\lambda)$ on the radius s is indicated explicitly. Hertel[11] observed that iterating Eq. (2.54) leads to a sequence of alternating bounds if one starts with an upper or lower bound to $\tilde{w}$. Numerical analysis of the iteration shows that a monotonic decreasing renormalized potential is incompatible with the obtained bounds. "From it upper and lower bounds to $n(\lambda)$ can be calculated which already after five iterations forbid a monotonic $n(\lambda)$. In these computations the numerical approximations were carefully done so that bounds really remained bounds" (quoted from Hertel[11]).

III. EXISTENCE OF A GRAVITATIONAL PHASE TRANSITION

In Sec. II we developed tools and results in the general Thomas–Fermi theory of a gravitational Fermi system, most of which enable us to prove in this section the appearance of at least two solutions in the Thomas–Fermi equation. For this purpose the properties of the temperature as function of the parameter ν are studied first, using results from Proposition 2.23.

Definition 3.1: Given the radius $R>0$, the normalization constant $n>0$, and a parameter $\nu\in\mathbb{R}$, the function $\beta:(R,n,\nu)\to\beta(\nu)\in\mathbb{R}_+$ is defined implicitly by

$$n = \beta(\nu)^{-3/4}\int_0^{\beta(\nu)^{-1/4}R} 4\pi\xi^2\, g(1,\xi^{-1}v(\xi)+\nu)\, d\xi \tag{3.1}$$

and $v(\xi)=v_1(\xi,\nu)$ is the solution of the λ-equation (2.42)–(2.45).

Remark 3.2: The roles of β and n are now exchanged. Always $R>0$ and $n>0$ is fixed from the beginning. We can speak of a β-equation instead of the n-equation. If this n- or β-equation has several different solutions $\rho_i(n,\beta,R)\in\bar{\Omega}$ $(i=1,2,\ldots)$, then there exist several different $\nu_i=\bar{\nu}[\rho_i(n,\beta,R)]$ (with $\nu=\beta\lambda$ and $\bar{\nu}=\beta\bar{\lambda}$) such that $\beta(\nu_i)=\beta$, i.e., $\beta(\nu)$ is a nonmonotonic function. Each $\rho_i(n,\beta,R)=\rho_{\nu_i}$.

Lemma 3.3: Given $R>0$, $n>0$, and let $\nu\in\mathbb{R}$. Then the function $\nu\to\beta(\nu)$ has the following properties:

(i) $\nu\to\beta^{-1}(\nu)$ is an entire real analytic function.

(ii) $\beta^{3/2}(\nu)\leqslant\frac{1}{3}(R^3/n)g(1,\nu)$.

Proof: (i) The function

$$\psi(y,\nu) = n - y^3R^{-3}\int_0^y 4\pi t^2 g(1,t^{-1}v(t,\nu)+\nu)\, dt \tag{3.2}$$

is analytic in $(y,\nu)\in(0,L_0)\times(-\nu_4,\nu_4)$ for arbitrary L_0, $\nu_4>0$, because

$$y^5\frac{d}{dy}(y^{-1}v(y)) = y^3\int_0^y 4\pi t^2\, g(1,t^{-1}v(t,\nu)+\nu)dt,$$

and v is analytic in $(0,L_0)\times(-\nu_4,\nu_4)$ by the proof of Proposition 2.23(i). Furthermore $\partial/\partial y\psi(y,\nu)\neq 0$ for all $(y,\nu)\in(0,L_0)\times(-\nu_4,\nu_4)$. Therefore, $\nu\to\beta^{-1}(\nu)$ is analytic by the implicit function theorem and (3.1) $(y=\beta^{-1/4}R)$.

(ii) follows trivially from $v(\xi)\geqslant 0$ and (3.1).□

Remark 3.3 (*iii*): Under the conditions of Lemma 3.3 there exist $R_0>0$, $n_0>0$ such that $\nu\to\beta(\nu)$ is not monotonic.

The *proof* relies on Remark 2.23(v) and is therefore not completely analytic:

By analyticity of $n(\nu)$, $\beta^{-1}(\nu)$, and $v(\xi,\nu)$ and with Lebesgue's theorem, differentiation of (3.1) with respect to $\nu\in(-\nu_4,\nu_4)$ leads to

$$\frac{\partial^{ex}}{\partial\nu}n(\nu,\beta(\nu),R) = A\cdot\frac{\partial}{\partial\nu}\beta(\nu) \tag{3.3}$$

with

$$A = \tfrac{3}{4}\beta^{-1}(\nu)\cdot n + \pi\beta^{-5/2}(\nu)R^3\, g(1,\epsilon(\nu,R,n)), \tag{3.4}$$

$$\epsilon(\nu,R,n) = \beta^{1/4}(\nu)R^{-1}\, v(\beta^{-1/4}(\nu)R,\nu)+\nu, \tag{3.5}$$

and with

$$\frac{\partial^{ex}}{\partial\nu}n(\nu,\beta,R) = \beta^{-3/4}\int_0^{\beta^{-1/4}R} d\xi\, 4\pi\xi^2$$
$$\times g'(1,\xi^{-1}v(\xi,\nu)+\nu)\left(1+\xi^{-1}\frac{\partial}{\partial\nu}v(\xi,\nu)\right) \tag{3.6}$$

denoting the partial derivative of $n(\nu,\beta(\nu),R)$ with respect to the explicit dependence on ν only.

By Remark 2.23(v) there exist $\beta_0>0$, $R_0>0$, and $\nu_0\in(-\nu_4,\nu_4)$ with

$$\frac{\partial^{ex}}{\partial\nu}n(\nu_0,\beta_0,R_0)>0.$$

If $n_0=n(\nu_0,\beta_0,R_0)$ is chosen, then $\beta(\nu_0)=\beta_0$ by (3.1) and (2.33) and monotonicity of $n(\nu,\beta,R)$ as a function of β^{-1}. Therefore there exist $R_0>0$, $n_0>0$, and $\nu_0>0$, and

$$\frac{\partial}{\partial\nu}\beta(\nu)\Big|_{\nu=\nu_0}>0$$

by $A>0$ and (3.3). But $\beta(\nu)$ cannot be everywhere strictly monotonic increasing because of Lemma 3.3 (ii).□

Remark 3.4: It is not sufficient to know only properties of $\nu\to n(\nu)$, but we had to infer from them the behavior of $\nu\to\beta(\nu)$, in order to draw conclusions from the β-dependence of the free energy. From the basic principles of quantum statistics and the fact that the free energy Φ is a limit of rescaled usual local free energies,[3,5] it is known (Ref. 12, 2.1.3,2.2.6,1.2.15,1.2.14) that the free energy function $\beta\to\beta\Phi(\beta,R,n)$ (see Definition 2.7) is concave in $\beta\in(0,\infty)$. Therefore the free energy $\Phi(\beta,R,n)$ is continuous in $\beta\in(0,\infty)$.

Lemma 3.5: Given $n>0$, $R>0$, and a sequence $\{\beta_i\}_{i\in\mathbb{N}}$, $\beta_i\in(0,\infty)$, of inverse temperatures converging to $\beta_0\in(0,\infty)$ for $i\to\infty$. Let $\{\rho(\beta_i)\}_{i\in\mathbb{N}}$, $\rho(\beta_i)\in\Omega^{(1)}_{\beta_i,R,n}$, be a sequence of solutions of the n-equation such that the strong limit (with respect to the $\mathscr{L}_\infty$-topology) of $\rho(\beta_i)$ $(i\to\infty)$ exists and is equal to $\rho_0\in\Omega^{(1)}_{B,R,n}=\bigcup_{i\in\mathbb{N}}\Omega^{(1)}_{\beta_i,R,n}$.

Then

$$\lim_{i\to\infty}F_\rho[\rho(\beta_i)](n,\beta_i,R) = F_\rho[\rho_0](n,\beta_0,R). \tag{3.7}$$

Proof: The first and second summand of the free energy functional (2.12) are stongly continuous functions on $(\Omega^{(1)}_{B,R,n},\|\cdot\|_\infty)$ by a straightforward generalization of Lemma 2.16. Only the third summand in (2.12)

$$F_\rho^3[\rho](\beta)=\beta^{-1}\int_\Lambda d^3x\int\frac{d^3p}{(2\pi)^3}$$
$$\times\ln(1+e^{-\beta(p^2+W[\rho](x)-\bar\mu[\rho])}) \tag{3.8}$$

depends explicitly on β. By partial integration

$$F_\rho^3[\rho](\beta)=(1/6\pi^2)\int_0^R 4\pi r^2\,dr\int_0^\infty \epsilon^{3/2}d\epsilon$$
$$\times(1+e^{\beta(\epsilon+\bar W[\rho](r)-\bar\mu[\rho])})^{-1}. \tag{3.9}$$

Let the smallest closed interval in $(0,\infty)$, which contains (almost) all of the elements of the above sequence $\{\beta_i\}_{i\in\mathbb{N}}$, be denoted by B. B is a compact set inside of $(0,\infty)$. Clearly there exist $\hat g_0>0$ and $\check\mu_0,\hat\mu_0\in\mathbb{R}$ such that, for each $\rho\in\Omega^{(1)}_{B,R,n}$, $0\leqslant\rho(x)\leqslant\hat g_0$ and $\check\mu_0\leqslant\bar\mu[\rho]\leqslant\hat\mu_0$. The estimate

$$|F_\rho^3[\rho_1](\beta_1)-F_\rho^3[\rho_2](\beta_2)|$$
$$\leqslant|\beta_1-\beta_2|C+D\{c_1\|\rho_1-\rho_2\|_\infty+|\bar\mu[\rho_1]-\bar\mu[\rho_2]|\} \tag{3.10}$$

for $\beta_1,\beta_2\in B$ and $\rho_1,\rho_2\in\Omega^{(1)}_{B,R,n}$ with

$$D=(\beta_4/6\pi^2)\int_0^R 4\pi r^2dr\int_0^\infty\epsilon^{3/2}d\epsilon I(\epsilon), \tag{3.11}$$
$$I(\epsilon)=(1+e^{\beta_3\epsilon-\beta_4(c_1\hat g_0+\hat\mu_0)})^{-1}, \tag{3.12}$$
$$C=E+(c_1\hat g_0+\hat\mu_0)\beta_4^{-1}D, \tag{3.13}$$
$$E=(1/6\pi^2)\int_0^R 4\pi r^2\,dr\int_0^\infty\epsilon^{5/2}\,d\epsilon\;I(\epsilon), \tag{3.14}$$

and continuity of $\bar\mu[\cdot]$ on $\Omega^{(1)}_{B,R,n}$ concludes the proof. Here $0<\beta_3<\beta_4$ have been chosen such that $B=[\beta_3,\beta_4]$.□

Lemma 3.6: Given $n>0$, $R>0$, and a sequence $\{\beta_i\}_{i\in\mathbb{N}}$, $\beta_i\in(0,\infty)$, of inverse temperatures converging to $\beta_0\in(0,\infty)$ for $i\to\infty$. Let $\{\rho(\beta_i)\}_{i\in\mathbb{N}}$, $\rho\in\Omega^{(1)}_{\beta,R,n}$ be a sequence of solutions of the n-equation and let $\nu_i=\beta_i\bar\lambda[\rho(\beta_i)]$. Suppose that $\lim_{i\to\infty}\nu_i=\nu_0$ exists, then on $(\Omega^{(1)}_{B,R,n},\|\cdot\|_\infty)$

$$s\text{-}\lim_{i\to\infty}\rho_{\nu_i,\beta_i}=\rho_{\nu_0,\beta_0} \tag{3.15}$$

exists, where $\rho_{\nu,\beta}$ denotes the (unique) solution of the λ-equation for temperature β^{-1} and $\nu=\beta\bar\lambda[\rho(\beta)]$, and B is defined as in Lemma 3.5.

Proof: Let us denote $\beta_i\,\tilde w(r)(\beta_i,\nu_i,R)=\bar w_i(r)$. Then the λ-equation is equivalent to the integral equation (2.54):

$$\bar w(r)=(K\bar w)(r)=\beta^{-1/2}\int_0^r s^{-2}\,ds\int_0^s dt\;4\pi t^2\,g(1,\nu+\bar w(t)). \tag{3.16}$$

On the cone $\mathscr{W}$ of positive, bounded, continuous functions $\mathbb{R}\to\mathbb{R}_+$ we introduce the metric[11]

$$d^\alpha(x,y)=\sup_{0\leqslant r\leqslant R}e^{-\alpha r}|x(r)-y(r)| \tag{3.17}$$

for $x,y\in\mathscr{W}$ and $\alpha>0$. $(\mathscr{W},d^\alpha)$ is a metric space for all $\alpha>0$. Note that

$$d^\alpha(K\bar w_i,K\bar w_0)\leqslant|\beta_i^{-1/2}-\beta_0^{-1/2}|d^\alpha(\tilde K\bar w_i,0)$$
$$+\beta_0^{-1/2}d^\alpha(\tilde K\bar w_i,\tilde K\bar w_0) \tag{3.18}$$

with $\tilde K\bar w=\beta^{1/2}K\bar w$ and $d^\alpha(\tilde K\bar w_i,\delta\tilde K\bar w_0)\leqslant\beta_4^{3/2}\frac{4}{3}\pi\hat g_0$ with $\delta\in\{0,1\}$ and $\beta_4,\hat g_0$ as in Lemma 3.5.

In particular the limit superior $\overset{(\sim)}{d}{}^\alpha_\delta=\overline{\lim_{i\to\infty}}\,d^\alpha(\overset{(\sim)}{K}\bar w_i,\delta\overset{(\sim)}{K}\bar w_0)$ exists. The second term in (3.18) has the following upper bound:

$$d^\alpha(\tilde K\bar w_i,\tilde K\bar w_0)\leqslant(1/\alpha^2)J_i\{|\nu_i-\nu_0|+d^\alpha(K\bar w_i,K\bar w_0)\}. \tag{3.19}$$

By Lebesgue's theorem and boundedness of $\{\nu_i\}$ and $\{\beta_i\}\subset B$ we can express $J_i=J(\nu_i,\beta_i,\nu_0,\beta_0)$ as

$$J_0=\lim_{i\to\infty}J_i=J(\nu_0,\beta_0,\nu_0,\beta_0), \tag{3.20}$$
$$J_0=(1/\pi)\int_0^\infty d\epsilon\;\sqrt{\epsilon}\,e^{\epsilon+\nu_0+\beta_0(2\pi/3)\hat g_0}/(1+e^{\epsilon+\nu_0})^2. \tag{3.21}$$

If α is chosen such that $J_0\beta_0^{-1/2}/\alpha^2=\epsilon_1<1$, then it follows from (3.18) and (3.19) that

$$d_1^\alpha\leqslant\epsilon_1 d_1^\alpha\leqslant\epsilon_1^k d_1^\alpha \tag{3.22}$$

for all $k\in\mathbb{N}$. Consequently, from (3.22)

$$0\leqslant d_1^\alpha\lim_{k\to\infty}(1-\epsilon_1^k)=d_1^\alpha\leqslant 0. \tag{3.23}$$

With $\rho_{\nu,\beta}=\beta^{-3/2}g(1,\nu+\bar w)$ we estimate

$$\|\rho_{\nu_i,\beta_i}-\rho_{\nu_0,\beta_0}\|_\infty\leqslant|\beta_i^{-3/2}-\beta_0^{-3/2}|\hat g_0$$
$$+(1/4\pi)\beta_0^{-3/2}J_i\{|\nu_i-\nu_0|+\|K\bar w_i-K\bar w_0\|_\infty\}. \tag{3.24}$$

The relations

$$d^\alpha(K\bar w_i,K\bar w_0)\geqslant e^{-\alpha R}\|K\bar w_i-K\bar w_0\|_\infty, \tag{3.25}$$

(3.23), and (3.24) lead finally to (3.15).□

Remark 3.7: From now on we assume that for each $\beta>0$, $R>0$, and $n>0$ there exists a unique solution $\rho_{\rm TF}$ of the Thomas–Fermi equation. By definition let $\nu_{\rm TF}(\beta)=\beta\bar\lambda[\rho_{\rm TF}(\beta)]$. This map $\beta\to\nu_{\rm TF}$ becomes a function because of the uniqueness of $\rho_{\rm TF}$.

Lemma 3.8: There exists a $\beta_0\in(0,\infty)$ and subsequences $\{\beta_{i_j}\}_{j\in\mathbb{N}}$, $\beta_{i_j}\in(0,\infty)$, and $\{\beta_{i_k}\}_{k\in\mathbb{N}}$, $\beta_{i_k}\in(0,\infty)$ converging to β_0 such that

$$\lim_{i_j\to\infty}\nu_{\rm TF}(\beta_{i_j})=\nu_1\neq\nu_2=\lim_{i_k\to\infty}\nu_{\rm TF}(\beta_{i_k}). \tag{3.26}$$

Proof: Let $\mathscr{M}$ denote the set of all local maxima of $\nu\to\beta(\nu)$ and $\mathscr{m}$ the set of all local minima of $\nu\to\beta(\nu)$. Then $\mathscr{M}\neq\emptyset$ and $\mathscr{m}\neq\emptyset$ by the nonmonotonicity and analyticity of $\nu\to\beta(\nu)$. Since $\nu\to\beta(\nu)$ is analytic, the extrema are isolated and have no accumulation points. The number of extrema is finite if ν is restricted to a compact set. Therefore, we can choose a local minimum and its neighboring local maximum. This pair can be chosen in a way such that there is no local minimum or local maximum between them. We can restrict our attention to the case where the local minimum is at $\nu_0^{(1)}$ and the local maximum at $\nu_0^{(2)}>\nu_0^{(1)}$, because, otherwise, when the local minimum is at $\nu_0^{(2)}$, the slope $d\beta/d\nu$ cannot stay always positive for $\nu>\nu_0^{(2)}$ because of Lemma 3.3 (ii), and there exists a local maximum at $\nu_0^{(3)}>\nu_0^{(2)}$ being next to the assumed local minimum at $\nu_0^{(2)}$. Note that $\beta(\nu)\to 0$

when $\nu \to \infty$ and that $\beta(\nu) \to \infty$ when $\nu \to -\infty$, because for each $\beta \in \mathbb{R}_+$ there has to exist a $\nu \in \mathbb{R}$ such that $\beta = \beta(\nu)$, as in Proposition 2.23 (iii). For ν's nearby to $\nu_0^{(1)}, \nu_0^{(2)}$ the domain of the map $\beta, \beta_{-1}(\nu)$ [i.e., $\beta \circ \beta_{-1} = \mathrm{id} \restriction (0,\infty)$] has necessarily at least three elements. One of them, $\nu_1 \in \beta_{-1}(\nu)$, is $\nu_1 = \nu_{\mathrm{TF}}(\beta_1)$ with $\beta(\nu_1) = \beta_1$, because to each $\beta_1 > 0$ there exists a (unique) ν_{TF} with $\beta_1 = \beta(\nu_{\mathrm{TF}})$. Now we assume

$$\beta \to \nu_{\mathrm{TF}}(\beta) \text{ is continuous for each } \beta \in (0,\infty). \tag{3.27}$$

We distinguish three cases: First case: $\nu_{\mathrm{TF}}(\beta_1) < \nu_0^{(1)}$. By continuity we can reach $\nu_0^{(1)}$ with $\nu_{\mathrm{TF}}(\beta(\nu_0^{(1)})) = \nu_0^{(1)}$. If we continue to values $\nu > \nu_0^{(1)}$, then $\beta(\nu) > \beta(\nu_0^{(1)})$ and the map $\beta \to \nu_{\mathrm{TF}}(\beta)$ would be multivalued, which contradicts the fact that $\beta \to \nu_{\mathrm{TF}}(\beta)$ is a function (Remark 3.7). Therefore, the function $\beta \to \nu_{\mathrm{TF}}(\beta)$ has to jump at $\beta(\nu_0^{(1)})$ to some value $\nu > \nu_0^{(2)}$ which contradicts (3.27). Second and third case: Assume $\nu_0^{(1)} < \nu_{\mathrm{TF}}(\beta_1) < \nu_0^{(2)}$; then the same argument as in the first case applies continuing either to $\nu_0^{(1)}$ or to $\nu_0^{(2)}$. In case $\nu_0^{(2)} < \nu_{\mathrm{TF}}(\beta_1)$ we have to continue to $\nu_0^{(2)}$. The contradictions to (3.27) obtained in all three cases prove Lemma 3.8 by analyticity of $\nu \to \beta(\nu)$ and the properties proved in Lemma 3.3, i.e., the discontinuity can only be a finite jump.□

Theorem 3.9: There exist $\beta > 0$, $R > 0$, and $n > 0$, such that the temperature-dependent Thomas-Fermi equation for gravitating fermions (Definition 2.7) has at least two solutions.

Proof: By Lemma 3.8 there exist a $\beta_0 > 0$ and subsequences $\{\beta_{i_j}\}_{j \in \mathbb{N}}, \beta_{i_j} \in (0,\infty)$, $\{\beta_{i_k}\}_{k \in \mathbb{N} \setminus \mathbb{I}}, \beta_{i_k} \in (0,\infty)$, converging to β_0 such that with Lemma 3.5, Lemma 3.6, Lemma 3.8, and Remark 3.4:

$$\begin{aligned} \lim_{i_j \to \infty} F_\rho\left[\rho_{\nu_{\mathrm{TF}}(\beta_{i_j}),\beta_{i_j}}(\beta_{i_j})\right] &= F_\rho\left[s - \lim_{i_j \to \infty} \rho_{\nu_{\mathrm{TF}}(\beta_{i_j}),\beta_{i_j}}\right](\beta_0) \\ &= F_\rho\left[\rho_{\nu_1,\beta_0}\right](\beta_0) = \lim_{i_j \to \infty} \Phi(\beta_{i_j}) = \Phi(\beta_0) = \lim_{i_k \to \infty} \Phi(\beta_{i_k}) \\ &= F_\rho\left[\rho_{\nu_2,\beta_0}\right](\beta_0). \end{aligned} \tag{3.28}$$

With Lemma 2.22 there exist two solutions of the Thomas–Fermi equation. This contradicts the assumption, made in Remark 3.7, that ρ_{TF} is unique for each $\beta > 0$, $R > 0$, and $n > 0$.□

As is well-known, the free energy Φ for gravitating fermions has special scaling properties.[3-5] Therefore, the point of phase transition (nonuniqueness of the solutions of the Thomas–Fermi equation) occurs not only at one point (β_0, R_0, n_0) but at a line where only two of the three thermodynamic parameters need to be fixed. For example, if (β_0, R_0, n_0) is a point where a phase transition occurs, then this phase transition shows up also at $(\gamma^{-4/3}\beta_0, \gamma^{-1/3}R_0, \gamma n_0)$ for all $\gamma > 0$. That the nonuniqueness of solutions of the Thomas–Fermi equation is connnected to a phase transition, and the nature of this phase transition can be seen from considering derivatives of the free energy Φ. If ρ_{TF} is unique then the first derivative:

$$\bar{\mu}[\rho_{\mathrm{TF}}] = \frac{\partial}{\partial n}\Phi(n,\beta,R) \tag{3.29}$$

exists.[4] In case of two solutions $\rho_{\mathrm{TF},1}$ and $\rho_{\mathrm{TF},2}$ we have $\Phi = F_\rho[\rho_{\mathrm{TF},1}] = F_\rho[\rho_{\mathrm{TF},2}]$ but with Lemma 2.22 $\bar{\mu}[\rho_{\mathrm{TF},1}] \neq \bar{\mu}[\rho_{\mathrm{TF},2}]$. Therefore the derivative in (3.29) cannot exist. Consequently, the nonuniqueness of the solutions of the Thomas–Fermi equation is equivalent to an Ehrenfest phase transition of the first kind in a system of gravitating fermions. This feature can also be observed by considering the mechanical pressure[4]

$$P[\rho] = -\frac{\partial}{\partial V}\Phi(n,\beta,R), \tag{3.30}$$

with $V = |\Lambda| = \frac{4}{3}\pi R^3$. Since[4]

$$P[\rho] = \tfrac{2}{3}\int \frac{d^3p}{(2\pi)^3} p^2 (1 + e^{\beta(p^2 - n/R - \bar{\mu}[\rho])})^{-1}, \tag{3.31}$$

the pressure becomes discontinuous and the derivative (3.30) does not exist at the phase transition point.

This phase transition has a remarkable nature, it is accompanied by an implosion or explosion respectively. In the framework of Thomas–Fermi theory of realistic matter models, the gravitating particles are the only ones to show a phase transition in the theory. For the ground-state Thomas–Fermi equation of ordinary matter, consisting of electrons (fermions) and nuclei (with infinite mass) interacting by Coulomb forces the solution is unique.[13,14] Uniqueness of the solutions holds also for the temperature-dependent Thomas–Fermi equation of ordinary matter.[15,16]

Note added in proof: In the meantime an analytical proof of the nonmonotonicity of the mass distribution as a function of the chemical potential was given. This closes our gap indicated at Remark 2.23(v). See J. Messer, "Non-Monotonicity of the Mass Distribution and Existence of the Gravitational Phase Transition," Phys. Lett. A **83**, 304 (1981).

ACKNOWLEDGMENTS

This work was started at the Institut für Theoretische Physik der Universität Göttingen at Göttingen, West Germany and continued at the Instituut voor Theoretische Fysica of the Universiteit Leuven at Leuven, Belgium. I am greatly indebted to Professor André Verbeure and all members of the theoretical physics group at Leuven for their generous hospitality. I am also grateful to Professor P. Hertel for pointing out an error in an earlier draft of the manuscript.

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The KMS condition and regularity for the ideal Bose gas

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(Received 10 March 1981; accepted for publication 5 June 1981)

We prove that the KMS condition for the infinite ideal Bose gas at any temperature $1/\beta$ and chemical potential $\mu \leqslant 0$ implies regularity under certain conditions on the test function space. Also, explicitly irregular solutions are constructed indicating the difference between the KMS condition and Gibbs states.

PACS numbers: 05.30.Jp

Let $\mathscr{D}$ be the set of complex infinitely differentiable functions with compact support in $\mathbb{R}^n$.

Define the one-parameter group $\{T_t\}_{t\in\mathbb{R}}$ of mappings:

$$T_t: \mathscr{D} \to \mathscr{D},$$

$$f \to T_t f = e^{it\epsilon} f,$$

where

$$\epsilon(k) = k^2/2 - \mu, \quad \mu \leqslant 0.$$

Let H by any T_t − invariant linear subspace of $\mathscr{D}$. We consider the *CCR-C* *-algebra: $\Delta(H,\sigma)$ over the test function space (H,σ), with $\sigma(f,g) = \mathrm{Im}\langle f,g\rangle$, where $\langle .,. \rangle$ denotes the usual L^2-scalar product.

The algebra is generated by the Weyl operators

$$\{W(f) | f \in H\}$$

with product and involution:

$$W(f)W(g) = W(f+g)e^{-i\sigma(f,g)/2},$$

$$W(f)^* = W(-f), \quad \forall f, g \in H.$$

(For more details see Ref. 1).

In this note, we consider the free Bose gas for which the time evolution is given by the one-parameter group $\langle \alpha_t \rangle_{t\in\mathbb{R}}$ of * − automorphisms on $\Delta(H,\sigma)$:

$$\alpha_t(W(f)) = W(T_t f), \quad \forall f \in H, \quad \forall t \in \mathbb{R}. \tag{1}$$

Definition (Ref. 2): A state ω on a C *-algebra $\mathscr{A}$ satisfies the KMS condition at inverse temperature $1/\beta$ with respect to a one parameter group $(\alpha_t)_{t\in\mathbb{R}}$ of *-automorphisms on $\mathscr{A}$ if, $\forall x, y \in \mathscr{A}$ there exists a function

$$F_{x,y}: \mathscr{C} \to \mathscr{C}$$

bounded and continuous on the strip $\{z \in \mathscr{C} | 0 \leqslant \mathrm{Im}\, z \leqslant \beta\}$ and analytic inside this strip, with boundary conditions

$$F_{x,y}(t) = \omega(x\alpha_t(y)),$$

$$F_{x,y}(t + i\beta) = \omega(\alpha_t(y)x).$$

In a well known paper,[3] Rocca, Sirugue, and Testard solved the KMS equation for quasi free evolutions, satisfying a number of conditions. (See also Ref. 4). They restricted the set of states to the so-called regular states in the sense of Segal, i.e., the set of states ω for which the map

$$\lambda \in \mathbb{R} \to \omega(W(\lambda f)W(g)) \in \mathscr{C}$$

is continuous for all $f, g \in H$.

Then it is well known that, if $(\pi_\omega, \mathscr{H}_\omega, \Omega_\omega)$ is the GNS triplet induced by the state ω, and if the state ω is regular, there exists a field $\mathscr{B}_\omega$, i.e., a map of H into the self-adjoint operators on the representation space $\mathscr{H}_\omega$, such that[1]

$$\pi_\omega(W(f)) = e^{i\mathscr{B}_\omega(f)}, \quad \forall f \in H.$$

One can ask the question whether the KMS condition already implies the regularity condition, such that the restriction made in Ref. 3 is unnecessary. One is tempted to conclude this question positively from the apparent analogy between the continuity of the function

$$\lambda \in \mathbb{R} \to \omega(W(\lambda f + g))$$

and the analyticity of the function

$$t \in \mathbb{R} \to \omega(W(T_t f + g)),$$

which follows from the KMS condition, as we prove in the next proposition.

Proposition 1: If ω is a KMS state at inverse temperature β on $\Delta(H,\sigma)$ with respect to the one-parameter group $\{\alpha_t\}_{t\in\mathbb{R}}$ defined in Ref. 1, then the mapping

$t \in \mathbb{R} \to \omega(W(T_t f + g))$ is analytic

for all $t \in \mathbb{R}$ and for all $f, g \in H$.

Proof: We note that for all $f, g \in H$

$$\omega(W(f)W(T_t g)) = \omega(W(T_t g)W(f))e^{-i\sigma(f,T_t g)}$$
$$= \omega(W(T_t g)W(f))$$
$$\times [\exp -(1/2)(\langle f, e^{it\epsilon} g\rangle - \langle e^{it\epsilon} g, f\rangle)].$$

Define

$$G_{f,g}(z) = F_{W(f),W(g)}(z)\exp(\tfrac{1}{2}(\langle f, e^{iz\epsilon} g\rangle - \langle g, e^{-iz\epsilon} f\rangle)),$$

where $F_{W(f),W(g)}$ is the analytic function as given by Definition 1. Furthermore define

$$\tilde{F}_{f,g}(z) = F_{W(f),W(g)}(z) \quad \text{if } 0 < \mathrm{Im}\, z \leqslant \beta$$
$$= G_{f,g}(z - i\beta) \quad \text{if } \beta < \mathrm{Im}\, z \leqslant 2\beta.$$

By construction this function is continuous in the strip $\{z \in \mathscr{C} | 0 \leqslant \mathrm{Im}\, z \leqslant 2\beta\}$ and analytic inside the strip: $\{z \in \mathscr{C} | 0 < \mathrm{Im}\, z < \beta\} \cup \{z \in \mathscr{C} | \beta < \mathrm{Im}\, z < 2\beta\}$. This implies that $\tilde{F}_{f,g}(z)$ is analytic in $\{z \in \mathscr{C} | 0 < \mathrm{Im}\, z < 2\beta\}$. In particular, the map $t \in \mathbb{R} \to \tilde{F}_{f,g}(t + i\beta)$ is analytic. Using $\tilde{F}(t + i\beta) = \omega(W(T_t f)W(g))$ and the commutation relations, we get the desired result. □

Although, Proposition 1 suggests that the KMS condition implies regularity in general, the situation is a bit more subtle. First, we take for H the following subspace of $\mathscr{D}$:

$$\text{or} \begin{matrix} H = \mathscr{D} & \text{if} & \mu < 0 \\ H = \{f \in \mathscr{D} | 0 \notin \mathrm{supp}\, f\} & \text{if} & \mu = 0 \end{matrix}. \tag{2}$$

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The idea of the next proposition is already contained in Ref. 3.

Proposition 2: If H is as in (2) and if ω is a KMS state of $\Delta(H,\sigma)$ at temperature $1/\beta$ with respect to the one-parameter group defined in (1), then $\exists\Phi: H\to C$ such that for all $f,g\in H$:

(i) $\omega(W(f)) = \Phi(f)$

$$\times\exp\{-\tfrac{1}{4}\int |f(k)|^2 \coth(\beta(k^2/2-\mu)/2)d^nk\},$$

(ii) $\Phi(T_t f+g) = \Phi(f+g) \quad \forall t\in\mathbb{R}$.

Proof: Let ω_1 be the linear functional of $\Delta(H,\sigma)$ defined by

$$\omega_1(W(f)) = \exp\{-\tfrac{1}{4}\int |f(k)|^2\coth(\beta(k^2/2-\mu)/2)d^nk\}.$$

It is easily verified that ω_1 is a KMS state of $\Delta(H,\sigma)$.
Define

$$\Phi(f) = \frac{\omega(W(f))}{\omega_1(W(f))}. \tag{3}$$

This is well defined since $\omega_1(W(f))\neq 0, \quad \forall f\in H$.
As ω and ω_1 are both KMS states and because of the special form of ω_1, it follows that

(a) $\Phi(T_t f+g)$ allows an analytic extension $\tilde{\Phi}(z)$ inside the strip $0\leqslant \mathrm{Im}\, z\leqslant\beta$, which is continuous on the strip,

(b) $\tilde{\Phi}(z)$ is bounded on this strip.

(c) $\tilde{\Phi}(t+i\beta) = \tilde{\Phi}(t)$.

Hence $\tilde{\Phi}(z)$ can be extended to a bounded function which is analytic on all $\mathcal{C}$, and hence by Liouville's theorem, $\tilde{\Phi}(z)$ is constant or

$$\Phi(T_t f+g) = \Phi(f+g), \quad \forall f,g\in H, \quad \forall t\in\mathbb{R} \qquad \blacksquare$$

Now we prove the main result about regularity.

Theorem 3: If the test function space H is taken as in (2), every KMS state of $\Delta(H,\sigma)$ for the free Bose gas at temperature $1/\beta$ is regular and hence assures the existence of a Bose field.

Proof: From Proposition 2, we have

$$\Phi(T_t f-f) = \Phi(0) = 1, \quad \forall f\in H, \quad \forall t\in\mathbb{R}, \tag{4}$$

where $\Phi(0) = 1$, since ω must be a state.

For all $g\in H$, define the function g_1 by

$$g_1(k) = \frac{g(k)}{e^{it_1(k^2/2-\mu)}-1}$$

with $0<t_1<\dfrac{\pi}{2\max\{k^2/2-\mu \mid k\in\mathrm{supp}\, f\}}$.

One checks that g_1 is well defined and that $g_1\in H$.
Take $t=t_1$ and $f=g_1$ in (4), then

$$\Phi((T_{t_1}-1)g_1) = \Phi(g) = 1, \quad \forall g\in H.$$

Thus, the unique KMS state on $\Delta(H,\sigma)$ at temperature $1/\beta$ is

$$\omega(W(f)) = \exp\{-\tfrac{1}{4}\int |f(k)|^2\coth\left(\beta\left(\frac{k^2}{2}-\mu\right)\Big/2\right)d^nk\},$$

which is regular. $\blacksquare$

Remark: One easily sees how this result can be generalized to other quasifree evolutions.

Consider a time evolution of the $\alpha_t(W(f)) = W(T_t f)$, where $(T_t f)(k) = e^{it\omega(k)}f(k)$ and with ω an infinitely differentiable function. Let $A = \{k\in\mathbb{R}^n \mid \omega(k)\leqslant 0\}$ and $H = \{f\in\mathscr{D} \mid \mathrm{supp}\, f\subset\mathbb{R}^n\setminus A\}$. Then, every KMS state of $\Delta(H,\sigma)$ for this quasifree evolution is regular.

Now we consider further the situation $\mu = 0$. We restrict our discussions to dimension $n\geqslant 3$. With minor changes the cases $n<3$ can be handled in the same way. We still have the possibility of choosing the test function space H:
Consider the following cases.

(a) $H=\mathscr{D}$. In this case it is easy to prove that there exist solutions of the KMS condition which are not regular. We give two examples:

The state ω_1 of $\Delta(\mathscr{D},\sigma)$ given by

$$\omega_1(W(f)) = \exp\{-\tfrac{1}{4}\int |f(k)|^2\coth(\beta k^2/4)d^nk\}$$

if $\mathrm{Re}\, f(0)$ is rational,

$$= 0 \quad \text{if } \mathrm{Re}\, f(0) \text{ is irrational.}$$

This is indeed verified to be a KMS state. However, it is easily seen to be not regular. Indeed take $f\in\mathscr{D}$ such that $\mathrm{Re}\, f(0)\neq 0$, then $\lambda\in\mathbb{R}\to\omega(W(\lambda f))$ is not continuous.
Another irregular state ω_2 is given by $f\in\mathscr{D}$,

$$\omega_2(W(f)) = \delta_{f(0),0}\exp\{-\tfrac{1}{4}\int |f(k)|^2\coth(\beta k^2/4)d^nk\},$$

where δ is the Kronecker symbol.
Here the discontinuity of

$$\lambda\in\mathbb{R}\to\omega_2(W(\lambda f))$$

is at $\lambda = 0$.
For these examples, it is clear that the irregularity shows up for all $f\in\mathscr{D}$ such that $\mathrm{Re}\, f(0)\neq 0$. It is well known that this quantity also describes the amount of condensation in the equilibrium states[5] and one may have the impression that condensation is responsible for the irregularity. This is not true, as follows from the next case.

(b) $H = \{f\in\mathscr{D} \mid f(0) = 0\}$. Let ω_3 be the following state:

$$\omega_3(W(f)) = \delta_{f'(0),0}\exp\{-\tfrac{1}{4}\int |f(k)|^2\coth(\beta k^2/4)d^nk\},$$

where

$$f'(0) = \left.\frac{\partial f(k)}{\partial k_1}\right|_{k=0} \text{ and } k = (k_1,\ldots,k_n).$$

In the notations of Proposition 2,

$$\Phi(f) = \delta_{f'(0),0}.$$

Again it is easily checked that the state ω is a KMS state but not a regular one. Take f such that $f'(0)\neq 0$, then

$\lambda\to\omega_3(W(f))$ is not continuous in $\lambda = 0$.

The existence of irregular solutions indicates that for the ideal Bose gas the KMS condition allows more solutions then the ones obtained from limit Gibbs states, which are easily shown to be regular.

ACKNOWLEDGMENTS

We thank Dr. A. Verbeure, Dr. M. Fannes, and J. Quaegebeur for useful remarks and stimulating discussions.

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Time development of Bose systems

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(Received 18 July 1980; accepted for publication 3 October 1980)

We investigate the dynamics of an infinite Bose system in C^*-algebraic description. The free time development is constructed under some conditions which are natural from a physical point of view. The properties of locally perturbed dynamics are discussed.

PACS numbers: 05.30.Jp, 02.10. + w

INTRODUCTION

Let Σ be a physical system (infinite) and $\mathscr{A}$ a quasilocal algebra associated with it. Thus $\mathscr{A} = \cup_\Lambda \mathscr{A}_\Lambda$, where $\mathscr{A}_\Lambda$ represents the algebra of Λ-local observables. We shall also assume that each $\mathscr{A}_\Lambda$ is equipped with a one-parameter group of automorphisms $\tau_t^\Lambda : \mathscr{A}_\Lambda \to \mathscr{A}_\Lambda$ and that this group descibes the time evolution for the region Λ.

It seems that one of the most important problems in nonrelativistic quantum statistical mechanics is the question of general conditions for the existence of the following limit: $\lim_\Lambda \tau_t^\Lambda A$, $A \in \cup_\Lambda \mathscr{A}_\Lambda$ and also the general characterization of this limit. The above limit procedure usually depends strongly on the physical properties of the system, e.g., the topology under which the limit can exist. If the above limit exists, in some sense, we shall say that the infinite system Σ has a time development.

At present, the question of description of the time development for continuous system is known only in exceptional cases, e.g., Bose systems have well described dynamics, in above sense for Gibbs states.[1]

The objective of the present paper is to study the description of the time development of an infinite Bose system for distinguished family of states. We recall that not each state on CCR algebra $\mathfrak{A}_N$ has a continuous time evolution. This paper splits naturally into several parts. In Sec. 1 details of our model and formulation of the main assumptions are presented. Section 2 is devoted to the description of the free time development. The main result of this section is that a free time development exists for primary, gauge invariant, locally normal states. Finally, in the last section we discuss the perturbations of time evolution and present some conclusions. It is shown that a bounded perturbed dynamics does not have "good behavior" with respect to quasilocal structure. This result is to be expected since we consider the nonrelativistic time evolution.

1. THE MODEL

Let $(N,(.,.))$ be a pre-Hilbert space; then the equation $\sigma(f,g) = \mathrm{im}(f,g)$, $f,g \in N$ defines a nondegenerate symplectic bilinear form on N. By $\mathfrak{A}_N$ we will denote the C^*-algebra generated by nonzero elements $W(f)$, $f \in N$, satisfying $W(-f) = W(f)^*$ and $W(f)W(g) = \exp\{-\frac{1}{2} i\sigma(f,g)\} W(f+g)$. Let M be a subspace of $\mathscr{L}^2(R^\nu)$ formed by the functions with compact support. If Λ is a bounded open set of $\mathbb{R}^\nu$ and $\mathfrak{A}_\Lambda$ is the C^*-subalgebra of $\mathfrak{A}_M$ generated by $\{W(f); f \in \mathscr{L}^2(\Lambda)\}$ then $(\mathfrak{A}_M \{\mathfrak{A}_\Lambda\}_{\Lambda \subset \mathbb{R}^\nu})$ forms a quasilocal algebra. (For an orientation on this subject we refer to Chapters II and V of the Bratteli, Robinson book.[2]) In order to describe the free evolution we must introduce the one-particle free Hamiltonian for each region Λ. Let H be the usual self-adjoint Laplacian operator $(H\phi)(x) = -\nabla_x^2 \phi(x)$. Next for each bounded open set $\Lambda \subset \mathbb{R}^\nu$ let H_Λ denote any self-adjoint extension of H restricted to the infinitely differentiable functions with support in Λ. There are many such extensions each of which corresponds to a choice of boundary conditions. The one parameter group $e^{iH_\Lambda t}$ represents the one-particle free time evolution for the region Λ in the Schrödinger picture. Moreover, one can deduce that the net of unitary groups $\{e^{iH_\Lambda t}\}$ converges strongly to the group e^{iHt}.[3]

Since unitary operator is also a symplectic one (for our definition of the symplectic form) the multiparticle free time evolution, for the region Λ, will be defined as follows: $W(e^{iH_\Lambda t} f) = \tau_t^\Lambda W(f)$, $f \in \mathscr{L}^2(\Lambda)$. The mapping $\tau_t^\Lambda(\cdot)$ can be extended to $\mathfrak{A}_\Lambda$ and in fact the extension $\tau_t^\Lambda(\cdot)$ is a one-parameter group of automorphisms but this group is not strongly continuous. Both statements are valid for each Λ.

Now let us fix for a moment an arbitrary region $\Lambda \subset \mathbb{R}^\nu$ and consider a state $\omega_\Lambda(\cdot)$ of $\mathfrak{A}_\Lambda$. It will be assumed that

(i) $\omega_\Lambda(\cdot)$ is normal w.r.t. the Fock representation, i.e., $\omega_\Lambda(A) = \mathrm{Tr}_{\mathscr{H}(\Lambda)}(\rho^\Lambda \Pi_F^\Lambda(A))$, where $(\mathscr{H}(\Lambda), \Pi_F^\Lambda(A), \Omega_F^\Lambda)$ denotes the GNS triple associated with the Fock state[4] $\omega_\Lambda^F(\cdot)$ for the region Λ and ρ^Λ is a density matrix on $\mathscr{H}(\Lambda)$. It should be remarked that each such state has a well-defined time evolution, e.g., the function $\mathbb{R} \ni t \to \omega_\Lambda(\tau_t^\Lambda(A))$ $A \in \mathfrak{A}_\Lambda$ is a continuous one. This normality condition essentially means that each bounded region of the space has a well-defined number of particles. Without this restriction the time evolution can exhibit strange phenomena.[5]

Next let us consider two regions Λ and Λ' such that $\Lambda' \supseteq \Lambda$ and corresponding states $\omega_{\Lambda'}(\cdot), \omega_\Lambda(\cdot)$. It will be assumed that:

(ii) $\omega_{\Lambda'}(A) = \omega_\Lambda(A)$ for all $A \in \mathfrak{A}_\Lambda$ $(\Lambda' \geqslant \Lambda)$. The meaning of this isotony condition is that the state of the infinite system is determined by a net $\{\rho^\Lambda\}$ of density matrices satisfying the compatibility conditions $\rho^\Lambda = \mathrm{Tr}_{\mathscr{H}(\Lambda' \setminus \Lambda)} \rho^{\Lambda'}$. It gives

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the possibility of definition of the state on the quasi-local algebra, i.e., $\omega(\cdot) = \lim_{\Lambda\to\infty}\omega_\Lambda(\cdot)$ exists on $\cup_\Lambda \mathfrak{A}_\Lambda$ and has a unique continuous extension to $\cup_\Lambda \mathscr{A}_\Lambda = \mathfrak{A}$. The conditions (i) and (ii) are however still too weak to give a time development for the Bose system. Therefore we add the following:

(iii) $\omega(\cdot) = \lim_\Lambda \omega_\Lambda(\cdot)$ is a primary state [i.e. $\Pi_\omega(\mathfrak{A}_M)''$ is a factor].

(iv) $\omega(\cdot)$ is a gauge invariant state, i.e., $\omega(\cdot)$ is invariant under the group of gauge transformations:

$$[0,2\pi] \ni \theta \to \tau_\theta(W(f)) = W(e^{i\theta}f) \quad f\in M.$$

The physical sense of the condition (iii) is that the system is in a pure thermodynamic phase (since each such state has a trivial algebra of infinity). One can consider that the gauge group represents inner symmetries of individual particles and one expects gauge-group dependent quantities to be macroscopically unobservable. This explains the reason for condition (iv).

2. FREE TIME DEVELOPMENT

The aim of this section is to prove the following theorem.

Theorem: *If a state $\omega(\cdot)$ of an infinite bose system Σ satisfies conditions (i),...,(iv) (described in Sec. 1), then the system Σ has well-defined free time development as a one-parameter weakly continuous group of automorphisms of the von Neumann algebra $\Pi_\omega(\mathfrak{A}_M)''$.*

Before starting with the proof we need some definitions and lemmas. Let us consider the state $\omega_\Lambda(\cdot), \Lambda\in\mathscr{T} = \{\Lambda; \Lambda$ is an open bounded subset of $\mathbb{R}^\nu\}$. By assumption (i) $\omega_\Lambda(A) = \mathrm{Tr}_{\mathscr{H}(\Lambda)}\rho^\Lambda \Pi_F^\Lambda(A)\ A\in\mathfrak{A}_\Lambda$. Hence there must exist a unitary operator W_Λ such that

$$W_\Lambda : \mathscr{H}_{\omega_\Lambda} \to \overline{\mathrm{Span}\,\{\aleph_0 \Pi_F^\Lambda(A)\eta^\Lambda; A\in\mathfrak{A}_\Lambda\}} \equiv \mathscr{K}_\Lambda \subseteq \aleph_0\mathscr{H}(\Lambda),$$

where we use the following: $(\mathscr{H}_{\omega_\Lambda}, \Pi_{\omega_\Lambda}(\cdot), \Omega_{\omega_\Lambda})$ is the GNS triple associated with the state $\omega_\Lambda(\cdot), \aleph_0\mathscr{H}(\Lambda) = \oplus_{i\in I}\mathscr{H}(\Lambda), \rho^\Lambda = \Sigma_i \eta_i^\Lambda \otimes \bar{\eta}_i^{\Lambda *}$ with $\eta_i^\Lambda \in \mathscr{H}(\Lambda)$ and $\Sigma_i \|\eta_i^\Lambda\|^2 < \infty$, $\aleph_0\Pi_F^\Lambda(A)\xi^\Lambda = \oplus_i \Pi_F^\Lambda(A)\xi_i^\Lambda$ for any $\xi^\Lambda \in \aleph_0\mathscr{H}(\Lambda)$. We also need the following mappings:

$$(1)\ V_{\Lambda'\Lambda}(\aleph_0\Pi_F^\Lambda(A)\eta^\Lambda) = \aleph_0\Pi_F^{\Lambda'}(A)\eta^\Lambda,$$

$$(2)\ \tilde{V}_{\Lambda'\Lambda}(\Pi_\omega^\Lambda(A)\Omega_\omega) = \Pi_\omega^{\Lambda'}(A)\Omega_\omega,\ \Pi_\omega^\Lambda \equiv \Pi_\omega|_{\mathfrak{A}_\Lambda},$$

$$(3)\ \phi_{\Lambda'\Lambda}(\aleph_0\Pi_F^\Lambda(A)) = \aleph_0\Pi_F^{\Lambda'}(A),$$

$$(4)\ \tilde{\phi}_{\Lambda'\Lambda}(\Pi_\omega^\Lambda(A)) = \Pi_\omega^{\Lambda'}(A),\ \Pi_\omega^\Lambda \equiv \Pi_\omega|_{\mathfrak{A}_\Lambda},$$

where in all the above definitions $A\in\mathfrak{A}_\Lambda$, $\Lambda'\geqslant\Lambda$ and $\Lambda', \Lambda\in\mathscr{T}$ Moreover, $\mathscr{H}_\omega^\Lambda$ will denote the following subspace:

$$\mathscr{H}_\omega^\Lambda = \overline{\mathrm{span}\,\{\Pi_\omega^\Lambda(A)\Omega_\omega; A\in\mathfrak{A}_\Lambda\}}.$$

Lemma 1: *The following inductive limits exist*:

$$\text{(i)}\ \lim_{\Lambda\to\infty}\{\mathscr{K}_\Lambda; V_{\Lambda'\Lambda}; \Lambda'\geqslant\Lambda; \Lambda', \Lambda\in\mathscr{T}\} = \mathscr{K}.$$

$$\text{(ii)}\ \lim_{\Lambda\to\infty}\{\mathscr{H}_\omega^\Lambda; \tilde{V}_{\Lambda'\Lambda}; \Lambda'\geqslant\Lambda; \Lambda', \Lambda\in\mathscr{T}\} = \mathscr{H}_\omega.$$

$$\text{(iii)}\ \lim_{\Lambda\to\infty}\{\aleph_0\Pi_F^\Lambda(\mathfrak{A}_\Lambda); \phi_{\Lambda'\Lambda}; \Lambda'\geqslant\Lambda; \Lambda', \Lambda\in\mathscr{T}\} = \Pi(\mathfrak{A}_M).$$

$$\text{(iv)}\ \lim_{\Lambda\to\infty}\{\Pi_\omega^\Lambda(\mathfrak{A}_\Lambda); \tilde{\phi}_{\Lambda'\Lambda}; \Lambda'\geqslant\Lambda; \Lambda', \Lambda\in\mathscr{T}\} = \Pi_\omega(\mathfrak{A}_M).$$

Moreover $(\mathscr{K}, \Pi(\mathfrak{A}_M))$ *is unitary equivalent to* $(\mathscr{H}_\omega, \Pi_\omega(\mathfrak{A}_M))$.

Proof: The mapping $V_{\Lambda'\Lambda}$ satisfies

$$V_{\Lambda''\Lambda'}V_{\Lambda'\Lambda} = V_{\Lambda''\Lambda}, \quad \Lambda''\geqslant\Lambda'\geqslant\Lambda$$

and it is an isometric embeding of $\mathscr{K}_\Lambda$ into $\mathscr{K}_{\Lambda'}(\Lambda'\geqslant\Lambda)$. Thus (i) follows from standard arguments of inductive limits. The analogous arguments give (ii), (iii), and (iv).

Next let us observe that $\mathscr{H}_\omega^\Lambda$ is unitary equivalent to $\mathscr{K}_\Lambda$, $(U_\Lambda(\Pi_\omega(A)\Omega_\omega) = \aleph_0\Pi_F^\Lambda(A)\eta^\Lambda; A\in\mathfrak{A}_\Lambda)$ and moreover the unitary mappings U_Λ satisfy compatibility conditions with mappings $V_{\Lambda'\Lambda}$ and $\tilde{V}_{\Lambda'\Lambda}$, i.e., $V_{\Lambda'\Lambda}U_\Lambda = U_{\Lambda'}\tilde{V}_{\Lambda'\Lambda}; \Lambda'\geqslant\Lambda$. Thus, there exists a unitary mapping U from $\mathscr{H}_\omega$ onto $\mathscr{K}$. Similar considerations and GNS representation theory give the last statement of Lemma 1.

Remark: We will denote by V_Λ (ϕ_Λ,...,etc) the canonical embending of $\mathscr{K}_\Lambda$ into $\mathscr{K}$, ($\aleph_0\Pi_F^\Lambda(\mathfrak{A}_\Lambda)$ into $\Pi(\mathfrak{A}_M)$,...,etc.). Moreover the explicit construction of inductive limits give the identification of $\Pi(\mathfrak{A}_M)$ as a subset of $B(\mathscr{K})$ [The same for $(\mathscr{H}_\omega, \Pi_\omega(\mathfrak{A}_M))$.] Also, for simplicity, we will denote $\Pi(W(f))$ by $W_\pi(f)$.

Lemma 2: *The following function*

$$M \supset \mathscr{L}^2(\Lambda) \ni f \to W_\pi(f) \in \Pi(\mathfrak{A}_M) \subseteq \mathscr{B}(\mathscr{K})$$

is continuous one when $\mathscr{L}^2(\Lambda)$ *is taken with the topology induced by the norm* $\|\cdot\|_{\mathscr{L}^2(\Lambda)} \equiv \|\cdot\|$ *whereas* $\mathscr{B}(\mathscr{K})$ *is equipped with the strong operator topology.*

Proof: First we observe that for an arbitrary $\Lambda\in\mathscr{T}$ and $f,g,h\in\mathscr{L}^2(\Lambda)$ $\|[\Pi_F^\Lambda(W(f)) - \Pi_F^\Lambda(W(g))]\,\Pi_F^\Lambda(W(h))\times\Omega_F^\Lambda\| \leqslant \|f-g\|\,\|h\|/4 + \|f-g\|\,\|f\|/4 + 2[1-\exp\{-\tfrac{1}{4}\|f-g\|^2\}]$. Hence, if $f_\alpha\to f$ then $\Pi_F^\Lambda(W(f_\alpha))\to\Pi_F^\Lambda(W(f))$. Now consider $\aleph_0\Pi_F^\Lambda(\cdot)$. Let ξ^Λ be in $\mathscr{K}_\Lambda$; then

$$\|\aleph_0\Pi_F^\Lambda(W(f_\alpha))\xi^\Lambda - \aleph_0\Pi_F^\Lambda(W(f))\xi^\Lambda\|^2$$

$$= \|\oplus_i [\Pi_F^\Lambda(W(f_\alpha))\xi_i^\Lambda - \Pi_F^\Lambda(W(f))\xi_i^\Lambda]\|^2$$

$$= \sum_i \|\Pi_F^\Lambda(W(f_\alpha))\xi_i^\Lambda - \Pi_F^\Lambda(W(f))\xi_i^\Lambda\|^2.$$

But by construction one can find, for each $\epsilon > 0$, an integer m such that

$$\sum_{i=m+1}^{\infty} \|\Pi_F^\Lambda(W(f_\alpha))\xi_i^\Lambda\|^2 < \frac{\epsilon}{3}$$

and

$$\sum_{i=m+1}^{\infty} \|\Pi_F^\Lambda(W(f))\xi_i^\Lambda\|^2 < \frac{\epsilon}{3}$$

uniformly in f_α and f. This result and the estimation for $\Pi_F^\Lambda(\cdot)$ imply that $\aleph_0\Pi_F^\Lambda(W(f_\alpha)) \xrightarrow{s} \aleph_0\Pi_F^\Lambda(W(f))$ if $f_\alpha\to f$ for f_α, f in $\mathscr{L}^2(\Lambda)$. Finally we estimate the following expression $\|[\Pi(W(f)) - \Pi(W(g))]x\|$, where $f,g\in M$, and $x\in\cup_\Lambda\{V_\Lambda\,\mathrm{Span}\{\aleph_0\Pi_F^\Lambda(A)\eta^\Lambda; A\in\mathfrak{A}_\Lambda\}\}$; i.e.,

$x\in V_{\Lambda_1}\,\mathrm{Span}\{\aleph_0\Pi^{\Lambda_1}{}_F(A)\eta^{\Lambda_1},A\in\mathfrak{A}_{\Lambda_1}\}$ for some Λ_1. Let $\Lambda\in\mathscr{T}$ and suppose Λ contains $\Lambda''\equiv\mathrm{supp}f$, $\Lambda'\equiv\mathrm{supp}g$ and Λ_1; then

$$\begin{aligned}\|[\Pi(W(f))-\Pi(W(g))]x\| &= \|[\phi_\Lambda\cdot\aleph_0\Pi^{\Lambda''}_F(W(f))-\phi_\Lambda\cdot\aleph_0\Pi^{\Lambda'}_F(W(g))]\\ &\quad\times V_{\Lambda_1}\aleph_0\Pi^{\Lambda_1}_F(A)\eta^{\Lambda_1}\|\\ &= \|[\phi_\Lambda\aleph_0\Pi^{\Lambda}_F(W(f))-\phi_\Lambda\aleph_0\Pi^{\Lambda}_F(W(g))]\\ &\quad\times V_\Lambda\aleph_0\Pi^{\Lambda}_F(A)\eta^{\Lambda}\|\\ &= \|V_\Lambda[\aleph_0\Pi^{\Lambda}_F(W(f))-\aleph_0\Pi^{\Lambda}_F(W(g))]\aleph_0\Pi^{\Lambda}_F(A)\eta^{\Lambda}\|\\ &= \|[\aleph_0\Pi^{\Lambda}_F(W(f))-\aleph_0\Pi^{\Lambda}_F(W(g))]\aleph_0\Pi^{\Lambda}_F(A)\eta^{\Lambda}\|,\end{aligned}$$

where we used the properties of inductive limits. In particular, the third equality follows from the compatibility in construction of inductive limits for $\mathscr{K}$ and $\Pi(\mathfrak{A}_M)$. The last estimation proves Lemma 2 because of the properties already established for $\aleph_0\Pi^{\Lambda}_F(\cdot)$.

Lemma 3: $\Pi_\omega(\mathfrak{A}_M)''$ contains a representation of the CCR algebra over $\mathscr{L}^2(\mathbb{R}^\nu)$ by the family of unitary Weyl operators.

Proof: Now we equip the space M with the topology induced by the norm $\|\cdot\|_{\mathscr{L}^2(\mathbb{R}^\nu)}\equiv\|\cdot\|$. It is easy to check that the assumptions of Theorem 2.6.10 in the book of Bratteli, Robinson[7] are also satisfied in our model [It is enough to study the lim $\{\aleph_0\Pi^{\Lambda}_F(\mathfrak{A}_\Lambda)'',\phi_{\Lambda'\Lambda};\Lambda'\geqslant\Lambda;\Lambda',\Lambda\in\mathscr{T}\}$, the mapping $\tau:\tau(\Pi^{\Lambda}_F(A))=\aleph_0\Pi^{\Lambda}_F(A)$ for $A\in\mathfrak{A}_\Lambda$ and to use Lemma 2.]

Therefore since by assumption $\omega(\cdot)$ is a primary state one can infer from the above cited theorem that for given Λ_0 and $\epsilon>0$, there exists a Λ' such that

$$|\omega(AB)-\omega(A)\omega(B)|\leqslant\epsilon\|A\|\|B\| \qquad (*)$$

for all $A\in\Pi_\omega(\mathfrak{A}_{\Lambda_0})''$, all $B\in\Pi_\omega(\mathfrak{A}_{\tilde\Lambda})''$ and all $\tilde\Lambda$ disjoint with Λ'. Let us define for each $f\in M$ the following net $f_\Lambda=\chi^\perp_\Lambda f$, where $\Lambda\in\mathscr{T}$,

$$\chi^\perp_\Lambda=\begin{cases}0, & x\in\Lambda\\ 1, & x\notin\Lambda\end{cases}.$$

$\{W_\pi(f_\Lambda)\equiv\Pi_\omega(W(f_\Lambda))\}$ is contained in the unit ball of $\mathscr{B}(\mathscr{H}_\omega)$ and this ball is weakly compact. It implies that there exists a subnet $\{W_\pi(f_\lambda)\}$ weakly convergent to $\mu 1$ (since the algebra at infinity is trivial). But then the condition (*) means for given $\Lambda_0\in\mathscr{T}$ and $\epsilon>0$ there exists an index λ' such that $\|E_{\Lambda_0}W_\pi(f_\lambda)\Omega_\omega-\mu\Omega_\omega\|<\epsilon$ for all $\lambda>\lambda'$. (E_{Λ_0} is the projector on the subspace $\overline{\mathrm{Span}}\{\Pi_\omega(A)\Omega_\omega;A\in\mathfrak{A}_{\Lambda_0}\}$.) This implies the strong convergence of $\{W_\pi(f_\lambda)\Omega_\omega\}$ and hence $|\mu|=1$. Moreover, by the gauge invariance of $\omega(\cdot)$,

$$\omega(W(f_\lambda)=\omega(W(e^{i\pi}f_\lambda))=\omega(W(-f_\lambda))=\omega(\overline{W(f_\lambda)})\to\mu.$$

Thus μ is a real number with absolute value 1. We must exclude the case $\mu=-1$. For this purpose let us observe that ±1 are unitary operators. This enables us to use properties of weak and strong operator topologies since these topologies coincide on the set of unitary operators. Let us assume that $W_\pi(f_\lambda)\to-1$ and consider $W_\pi((1/m)f_\lambda)$ where m is a large positive integer. Let us take a subnet of $W_\pi((1/m)f_\lambda)$ which we denote by $W_\pi((1/m)f_\alpha)$, such that $W_\pi((1/m)f_\alpha)$, is convergent [This is possible because $\{W_\pi((1/m)f_\alpha)\}$ is contained in the unit ball of $\mathscr{B}(\mathscr{H})_\omega$.] Our assumption, the equality

$W_\pi(f_\alpha)=W((1/m)f_\alpha)\cdots W((1/m)f_\alpha)$ and the coincidence strong and weak convergence of unitaries to a unitary limit exclude the possibility $W_\pi((1/m)f_\alpha)\to1$. The second case $W_\pi((1/m)f_\alpha)\to-1$ is impossible one since $\omega(\cdot)$ is a regular state[8] and $\omega(W(0))=+1$. Therefore $W_\pi(f_\lambda)\overset{s}{\to}+1$. Now let us consider the following inequality (for an arbitrary ψ):

$$\begin{aligned}\|(W_\pi(f_\Lambda)-1)\psi\|&\leqslant\|(W_\pi(f_\lambda)-1\psi\|\\ &+\|(W_\pi(f_\Lambda)-W_\pi(f_\lambda))\psi\|,\end{aligned}$$

where $\{W_\pi(f_\lambda)\}$ indicates a subnet of $\{W(f_\Lambda)\}$ and $\lambda\geqslant\Lambda\geqslant\lambda'$ (the last inequalities follow from the definition of subnet). From the construction of f_Λ,

$$\|f_\Lambda\|_{\mathscr{L}^2(\mathbb{R}^\nu)}\overset{\Lambda\to\infty}{\to}0 \quad\text{so that}\quad \|f_\lambda-f_\Lambda\|_{\mathscr{L}^2(\mathbb{R}^\nu)}\overset{\lambda'\to\infty}{\to}0.$$

Moreover, $f_\lambda-f_\Lambda$ is a function defined on a bounded region. Thus the convergence of $\{W_\pi(f_\lambda)\}$ and Lemma 2 imply $W_\pi(f_\Lambda)\overset{s}{\to}1$. To end the proof of Lemma 3 let us take an arbitrary $\tilde f\in M$ with $\|f\|_{\mathscr{L}^2(\mathbb{R}^\nu)}<\epsilon$.

One can decompose $\tilde f$ in the following way: $\tilde f=\tilde f_\Lambda+\tilde f_{\Lambda^\perp}$, where $\tilde f_\Lambda=\chi_\Lambda\tilde f\tilde f_{\Lambda^\perp}=\chi_{\Lambda^\perp}\tilde f$. ($\chi_\Lambda$ is a characteristic function of the region Λ). It is clear that $\|\tilde f\|_{\mathscr{L}^2(\mathbb{R}^\nu)}\geqslant\|\tilde f\|_{\mathscr{L}^2(\Lambda)}$, thus application of the previous arguments to the function $\tilde f_{\Lambda^\perp}$ and application of Lemma 2 to the function $\tilde f_\Lambda$ completes the proof of Lemma 3.

Proof of theorem: Let us define the following mapping:

$$\tau^0_t(W_\pi(f))=W_\pi(e^{iHt}f)\quad\text{for } f\in M. \qquad (**)$$

In general, due to instantaneous wave-spreading phenomena, $e^{iHt}f\in\mathscr{L}^2(\mathbb{R}^\nu)$. Lemma 3 however allows such a definition in $\Pi_\omega(\mathfrak{A}_M)''$. Let us denote by $\mathscr{A}_1$ (resp. $\bar{\mathscr{A}}_1$) the unit ball in $\mathscr{A}=\{\Sigma^l_1 c_iW_\pi(f_i);f_i\in M,c_i\in\mathbb{C}\}$ (in $\bar{\mathscr{A}}=\mathscr{A}''=\Pi_\omega(\mathfrak{A}_M)''$). For each $A\in\bar{\mathscr{A}}_1$ define

$$\tau_t(A)=\text{strong*}\lim\tau^0_t\Big(\sum_1^n a_iW_\pi(f_i)\Big),$$

where $\Sigma^n_1a_iW_\pi(f_i)\in\mathscr{A}_1$ is chosen to converge to A. (This is possible by Kaplansky's theorem.) The extension of $\tau_t(\cdot)$, by linearity, to $\bar{\mathscr{A}}$ will be denoted by the same symbol. Since the strong*-topology is compatible with the algebraic structure on the unit ball it is evident that $\tau_t(\cdot)$ is a one parameter family of *-homomorphisms. Let us denote by $\ker\tau_t$ the kernel of $\tau_t(\cdot)$ It is two sided ideal in $\bar{\mathscr{A}}$. Let us take the strong* (or equivalently weak) closure. We will denote this closure by $\overline{\ker\tau_t}$. Thus $\overline{\ker\tau_t}$ is weak-closed two-sided ideal in von Neumann algebra. Hence $\overline{\ker\tau_t}=\bar{\mathscr{A}}z$, where z is a central projection. Since $\omega(\cdot)$ is a primary state $z\in\{0,1\}$. Therefore the assumption that $\overline{\ker\tau_t}\neq\{0\}$ implies that the kernel $\tau_t(\cdot)$ is strong* dense in $\bar{\mathscr{A}}$. Let us assume this case, i.e. $\ker\tau_t\neq\{0\}$, and take an arbitrary $A\in\bar{\mathscr{A}}_1$. The assumption (ii) implies that $\bar{\mathscr{A}}$ is σ-finite von Neumann algebra acting on separable Hilbert space. Thus the strong*-topology on the $\bar{\mathscr{A}}_1$ is metrizable.[9] But Kaplansky's theorem there exists a sequence $A_n\in\ker\tau_t\cap\bar{\mathscr{A}}_1$ such that $A_n\overset{s^*}{\to}A$. On the other hand, also by Kaplansky's theorem, there exists for each n a

sequence

$$B_{n,m} = \sum_{i=1}^{l_{n,m}} c_{n,i} W_\pi(f_{n,i})$$

such that $B_{n,m} \in \mathscr{A}_1$ and $B_{n,m} \xrightarrow{s^*} A_n$. Since the strong*-topology is given by metric $\rho(\cdot)$ (on the unit ball) it is possible to pick the special subsequence B_{n_i,m_i} such that $B_{n_i,m_i} \xrightarrow{s^*}$ and for large enough indices (n_i,m_i) AB_{n_i,m_i} is arbitrarily close to A_{n_i}. But it implies that $\rho(\tau_t(A),0)$ is an arbitrarily small number and hence $A \in \ker\tau_t$. Thus $\mathscr{A} \subset \ker\tau_t$ what is not possible since, for example, $W_\pi(f)$ and $W_\pi(e^{iHt}f)$ are unitary operators. Therefore $\ker\tau_t = \{0\}$ and $\tau_t(\cdot)$ is a one-parameter family of automorphisms of the von Neumann algebra $\mathscr{A}$. Application of the fact that each automorphism of a von Neumann algebra is strong*-continuous on the unit ball[10] gives the result that $\tau_t(\cdot)$ is one-parameter group of automorphisms. Finally, $e^{iH_\lambda t} \xrightarrow{s} e^{iHt}$, and Lemma 3 gives an explanation of the name free time development.

3. PERTURBED TIME DEVELOPMENT

In this section we consider locally perturbed time developments τ^P on $\mathfrak{A}_\pi(\mathfrak{A}_M)''$. These evolutions are defined by the following formula:

$$\tau_t^P(A) = \tau_t(A) + \sum_{n\geq 1} i^n \int_{0\leq s_1\leq\cdots\leq s_n\leq t} ds_1\cdots ds_n \times [\tau_{s_n}(P),\cdots[\tau_{s_1}(P),\tau_t(A)]\cdots]$$

for $t\geqslant 0$, $P = P^*$; $A,P \in \Pi_\omega(\mathfrak{A}_M)''$. Analogous formulas hold for negative times. In this definition, the integrals are defined in the strong topology so they give elements in von Neumann algebra $\Pi_\omega(\mathfrak{A}_M)''$. Moreover, one can easily check that $\tau_t^P(\cdot)$ is a one-parameter group of automorphisms of $\Pi_\omega(\mathfrak{A}_M)''$.[11] In particular

$$\tau_t^P(A) = \mathrm{Exp}_r\left(\int_0^t ;iP(s)\,ds\right)\tau_t(A)\mathrm{Exp}_l\left(\int_0^t ; -iP(s)\,ds\right),$$

where

$$\mathrm{Exp}_r\left(\int_0^t ;iP(s)\,ds\right) = \sum_{n\geq 0} i^n \int_0^t dt_1\cdots\int_0^{t_{n-1}} dt_n\ \tau_{t_n}(P)\cdots\tau_{t_1}(P),$$

$$\mathrm{Exp}_l\left(\int_0^t ;iP(s)\,ds\right) = \sum_{n\geq 0} i^n \int_0^t dt_1\cdots\int_0^{t_{n-1}} dt_n\ \tau_{t_1}(P)\cdots\tau_{t_n}(P),$$

and

$$\mathrm{Exp}_r\left(\int_0^t ;iP(s)\,ds\right)^* = \mathrm{Exp}_l\left(\int_0^t ; -iP(s)\,ds\right).$$

Let us consider the following problem: Is it possible to define a locally perturbed evolution which preserves the C^*-algebraic structure? In other words, can one find $\tau_t^P(\cdot)$ with the property that $\tau_t^P(\Pi_\omega(\mathfrak{A}_M)) = \Pi_\omega(\mathfrak{A}_M)$. This question seems to be too general and a serious hint can be extracted from Kadison's corollary 4.6.[12] Namely let us define a w*-unimorphism to be an affine isomorphism continuous with respect to the w*-uniform structure, acting on convex compact uniform space S. [The w*-uniform structure is induced by weak*-topology since $S \subset X^*$ in our problem where X is a Banach space. In this section weak topology means $\sigma(X^*,X)$ topology in the sense of Banach space language].

The mapping $\tau_t^P(\cdot)$ has the desirable property if and only if the dual map $(\tau_t^P)^*$ is w*-unimorphism on the set of weak-operator continuous states. Since $\tau_t(\cdot)$ does not have the cited property, then $\mathrm{Exp}_r(\int_0^t ;iP(s)\,ds)$ does not induce a w*-unimorphism if $\tau_t^P(\cdot)$ preserves the C^*-algebraic structure. (We recall that the composition of two uniformly continuous functions is continuous.) Therefore the question posed is similar to the following one: When does the superposition of two 1–1, onto, not continuous functions give a continuous function? The following equality shows the whole difficulty: $h\circ f^{-1}\circ f = h$ for h continuous function and f discontinuous. The above arguments explain why we modify the posed problem to the following one: Is it possible to find nonexceptional bounded perturbation P such that $\tau_t^P(\cdot)$ preserves the C^*-algebraic structure. Nonexceptional perturbation means that $\tau_t^{(1+\lambda)P}$ preserves the structure for small $\lambda \in (-\epsilon,\epsilon)$.

Theorem: *It is not possible to find nonexceptional bounded perturbations P such that $\tau_t^P(\cdot)$ preserves quasilocal structure.*

Proof: Let us assume that a nonexceptional perturbation P exists. One has[13]

$$\tau_t^{(1+\lambda)P}(A) = \mathrm{Exp}_r\left(\int_0^t ;i(1+\lambda)P(s)\,ds\right)\tau_t(A)[\mathrm{Exp}_r(\cdots)]^*$$

$$= \mathrm{Exp}_r\left(\int_0^t ;(iP\mathbin{\dot{\wedge}}i\lambda P)(s)\,ds\right)\mathrm{Exp}_r\left(\int_0^t ;iP(s)\,ds\right)\tau_t(A) \times [\mathrm{Exp}_r(\cdots)\mathrm{Exp}_r(\cdots)]^*,$$

where

$$(B\mathbin{\dot{\wedge}}A) = \mathrm{Exp}_r\left(\int_0^t ;B(s)\,ds\right)\tau_t(A)\left[\mathrm{Exp}_r\left(\int_0^t ;B(s)\,ds\right)\right]^*.$$

Hence,

$$\mathrm{Exp}_r\left(\int_0^t ;(iP\mathbin{\dot{\wedge}}i\lambda P)(s)\,ds\right)(\cdot)\mathrm{Exp}_r\left(\int_0^t ;(iP\mathbin{\dot{\wedge}}i\lambda P)(s)\,ds\right)^* \equiv \beta(\cdot)$$

induces in the dual space a w^*-unimorphism. [In what follows, for simplicity, such $\mathrm{Exp}_r(\cdots)$ will be called w^*-unimorphism.] Propositions 6 and 9 of Ref. 14 imply that $\mathrm{Exp}_r(\int_0^t ;\{i(1+n\lambda)P\mathbin{\dot{\wedge}}(-i\lambda P)\}(s)\,ds)$ is w^*-unimorphism for $\lambda \in (-\epsilon,+\epsilon)$ and $n \in \mathscr{N}$. The following equalities give the basic idea of the proof of the above result:

$$\mathrm{Exp}_r\left(\int_0^t ;\{(1+\lambda)iP\mathbin{\dot{\wedge}}(-\lambda iP)\}(s)\,ds\right) \times \mathrm{Exp}_r\left(\int_0^t ;\{(iP\mathbin{\dot{\wedge}}i\lambda P)(s)\,ds\right)$$

$$= \mathrm{Exp}_r\left(\int_0^t ;\{(iP\mathbin{\dot{\wedge}}i\lambda P)\mathbin{\dot{\wedge}}(iP\mathbin{\dot{\wedge}}(-i\lambda P))\}(s)\,ds\right) \times \mathrm{Exp}_r\left(\int_0^t ;(iP\mathbin{\dot{\wedge}}i\lambda P)(s)\,ds\right) = I.$$

Thus one can choose $\delta \in (0,\epsilon)$ such that

$$\mathrm{Exp}_r\left(\int_0^t ;(0\mathbin{\dot{\wedge}}i\delta P)(s)\,ds\right) = \mathrm{Exp}_r\left(\int_0^t ;i\delta P(s)\,ds\right)$$

is a w^*-unimorphism.

Then the cited properties of the perturbed dynamics, properties of $\mathrm{Exp}_r(\cdot)$ and $\mathrm{Exp}_l(\cdot)$ imply that $\tau_t^{\delta p}(\cdot)$ does not preserve the C^*-algebraic structure. Moreover, δ can be chosen as a very small number. Let us call $\tau_t^1(\cdot) \equiv \tau_t^{\delta p}(\cdot)$ and repeat the above arguments, etc. The result is: $\tau_t^{Qp}(\cdot)$ does not preserve the C^*-algebraic structure where $Q = \delta + \delta(1-\delta) + \delta(1-\delta-\delta(1-\delta)) + \cdots$. Therefore, for appropriate choice of δ, one can make Q arbitrary close to 1 which is a contradiction.

ACKNOWLEDGMENTS

I am very grateful to D. W. Robinson for his hospitality at the School of Mathematics of the University of New South Wales where parts of this investigation were carried when the author was research fellow of A.R.G.C. I would like to thank also O. Bratteli and D. W. Robinson for their interest in this work, helpful discussions and critical comments. The grant of A.R.G.C. is gratefully acknowledged.

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[3] See example 3.1.29 in Chap. 3 of Ref. 2.
[4] The Fock state $\omega_\Lambda^F(\cdot)$ is defined by the formula $\omega_F^\Lambda(W(f)) = \exp\{-\frac{1}{4}\|f\|^2\}$, $f \in \mathscr{L}^2(\Lambda)$.
[5] Ch. Radin, Commun. Math. Phys. **54**, 69 (1977).
[6] Let X be a Hilbert space and $x,y \in X$. Then the operator $x \otimes \bar{y}$ is defined by the formula $(x \otimes \bar{y})z = (z,y)x$ for every $z \in X$.
[7] See Ref. 2.
[8] $\omega(\cdot)$ is a regular state if the following function $\mathbb{R} \ni a \to \omega(W(af))$ is continuous one for arbitrary f. This property follows from assumptions (i) and (ii).
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[13] See Prop. 6 cited in Araki's paper.
[14] Cited in Araki's paper.

The kinetic analog of Boltzmann's principle

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(Received 24 February 1981; accepted for publication 12 June 1981)

A general expression for the transition density of nonequilibrium diffusion processes is derived that is valid for non-Gaussian fluctuations. Using the thermodynamic principle, that relates the relative probability density of paths for absolutely continuous diffusion processes to the thermodynamic force, the kinetic analog of Boltzmann's principle is derived. The transition density can be expressed in terms of the difference in entropies of the endpoints of the transition and the joint entropy. The gradient of the joint entropy is a measure of the strength of statistical correlations between nonequilibrium states and its difference (sum) between the thermodynamic forces determines the rates of growth (decay) of fluctuations. These rates are mirror images in time of one another and display a symmetry in past and future. The macroscopic laws of irreversible thermodynamics emerge in the exact balance of these two phenomena.

PACS numbers: 05.40. + j, 05.70.Ln

I. INTRODUCTION AND SUMMARY

The search for a kinetic analog of Boltzmann's principle began with Onsager[1] and Onsager and Machlup.[2] Boltzmann's principle relates the probability of a spontaneous fluctuation from equilibrium to its entropy. When dealing with irreversible thermodynamic processes, it is important to know not only the distribution in the density of states but also the distribution in the density of paths connecting nonequilibrium states. Although Onsager and Machlup[2] introduced the novel feature of evaluating statistical distributions by variational expressions and provided a statistical interpretation of the dissipation function, their analysis was based on the Gaussian assumption and lacked the essential elements which ultimately lead to the establishment of the limiting statistical distribution. In other words, (i) the Gaussian assumption is at the root of the variational analysis of statistical distributions and cannot be generalized to non-Gaussian processes and (ii) the inclusion of random perturbations which generate statistical correlations between nonequilibrium states requires the use of stochastic rather than ordinary calculus.

Recent attempts to generalize the Onsager–Machlup formulation, either in terms of path integrals[3–7] or by probabilistic approaches,[8,9] have not led to any general thermodynamic principles for non-Gaussian, diffusion processes. Moreover, thermodynamic theories which emphasize the distinction between irreversible thermodynamic processes that occur near and far from equilibrium[10,11] in relation to their stability properties[12,13] fail, even in the near equilibrium regime, to obtain the necessary compatibility with equilibrium statistical thermodynamics in the asymptotic time limit where the statistical correlations between nonequilibrium states have worn of.[14,15]

In this article, we consider the general problem of the transformation of one diffusion process into another by means of an externally applied constraint which is then suddenly released. A general thermodynamic principle relates the restoring or thermodynamic force produced by the constraint to the relative distribution in the density of paths of the transformed or biased diffusion process with respect to the initial or unbiased diffusion process.

From this thermodynamic principle we obtain a general expression for the density of the probability measure of the biased diffusion process with respect to the probability measure of the set of paths belonging to the unbiased diffusion process. Averaging this expression over all paths connecting two given nonequilibrium states yields an expression for the transition density. Several interesting forms of the transition density are given.

In the first place, it can be expressed as a conditional Wiener integral of the so-called Onsager–Machlup potential.[16] Its relationship with the kernel that is essentially responsible for the propagation of the probability density in space-time is given and the associated eigenvalue problem is formulated. Although we leave the implied stability analysis, in terms of the Onsager–Machlup potential, for a separate publication,[17] it is interesting to note that stability considerations have already been applied to the Onsager–Machlup potential in the case where it has the form of a bistable potential well.[18]

In the second place, the transition density is shown to be completely determined by the difference in entropies of the endpoints of the transition and the joint entropy, which is a quasithermodynamic quantity that describes the statistical correlations between nonequilibrium states. This is the kinetic analog of Boltzmann's principle. The thermodynamic additive properties, that are characteristic of equilibrium statistical thermodynamics, are destroyed by the presence of statistical correlations between nonequilibrium states. It is only when a long enough time has elapsed, so as to have given the statistical correlations ample time to have worn off, that we regain statistical independence; the joint entropy reduces to the sum of the entropies of the given nonequilibrium states.

The gradient of the joint entropy is a measure of the

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strength of the statistical correlations. It provides information on the rates of growth and decay of fluctuations in irreversible thermodynamics processes that is not contained in the macroscopic, phenomenological laws. Furthermore, we show that macroscopic phenomenological laws arise from the sum of these two phenomena. This result is not based on the Gaussianity of the irreversible process. In fact, it is a generalization of the symmetry property in past and future that was found in Gaussian processes.[2,19]

The difference and sum of the gradients of the joint entropy and entropy are proportional to transitional velocities, which are the rates at which fluctuations grow and decay in irreversible thermodynamic processes, respectively. The sum of the transitional velocities is the thermodynamic flux that appears in the macroscopic phenomenological force-flux relations. This is to say that the macroscopic laws of irreversible thermodynamics arise by an exact balancing of the rates at which fluctuations grow and decay.

The rate of growth of fluctuations is related to the probability flux density of the forward Fokker–Planck equation for the transition density. Written in the form of continuity equation, it shows that the motion behaves as a compressible fluid. In the specific example of the Ornstein–Uhlenbeck process, the fluid compressibility is shown to be related to the velocity at which the distribution spreads. This factor, whose time rate-of-charge is proportional to the divergence of the transitional velocity for the growth of fluctuations, is seen to arise from the inherent uncertainty in position and velocity measurements of the Brownian particle. It is not possible to measure, with arbitrary precision, any two nonequilibrium states through which the system passes at successive instants in time, for it would be equivalent to a precise knowledge of the initial position and velocity of the Brownian particle. This is reflected in a nonvanishing value of the divergence of the rate at which fluctuations grow.

Potential conditions that would govern the behavior of irreversible thermodynamic processes have been proposed.[20] The transitional velocity for the decay of fluctuations is seen to satisfy a compatibility condition which expresses it as the gradient of the transition density. Since the transition density cannot be expressed solely in terms of a difference in a thermodynamic function of state, there can be no potential condition attached to the rate of decay of fluctuations. Only in the asymptotic time limit, where all statistical correlations have worn away, can the rate of decay of fluctuations be derived from a velocity potential. The compatibility condition then becomes the well-known Einstein condition for dynamic equilibrium which together with Boltzmann's principle identify the entropy as the velocity potential.

II. TRANSFORMATION OF DIFFUSION PROCESSES

Consider an unbiased Brownian motion to which we apply an external constraint.[21] The applied constraint can be an external electromotive force, a difference in temperature, etc. A thermodynamic force is produced which, when the constraint is suddenly removed, drives the system back to equilibrium. This constitutes a particular case of the transformation of one diffusion process into another, which are absolutely continuous with respect to one another. A necessary and sufficient condition for the absolute continuity of the probability measures is that the diffusion coefficients of the two processes be equal. However, the thermodynamic forces, which are proportional to the drift parameters of the diffusion processes, are different. The transformation of one diffusion process into another, both of which have a nonvanishing thermodynamic force, constitutes a generalization of the theory to nonequilibrium stationary states that we shall discuss below.

In the case that the reference state is thermodynamic equilibrium, an external constraint is applied to the unbiased Brownian motion

$$dX(t) = \sigma\, dW(t), \tag{1}$$

which converts it into a biased Brownian motion

$$d\tilde{X}(t) = L\chi(\tilde{X}(t))dt + \sigma\, dW(t) \tag{2}$$

after the constraint has been suddenly released. The absolute continuity of the two diffusion processes $X(t)$ and $\tilde{X}(t)$ is ensured by the fact that they have the same variance parameter σ. The assumption of a constant variance parameter is a simplification that does not lead to any loss of generality.[22] $W(t)$ is a Wiener process; that is, a process with independent increments. Its mathematical expectation is zero so that process (2) describes, on the average, the macroscopic phenomenological behavior that is dictated by the laws of irreversible thermodynamics. Correlations between the Wiener process in different instants in time are equal to the time that has elapsed. The externally applied constraint produces a thermodynamic force χ which acts as the restoring force when the constraint is suddenly removed. Note that we do not restrict it to be a linear function of the process; that is, we do not make the Gaussian assumption. Finally, the transport coefficient L is related to the diffusion coefficient according to Einstein's formula $L = \frac{1}{2}\sigma^2$ in units where Boltzmann's constant is equal to unity.

It now follows that the probability measures μ_W and μ_T associated with diffusion processes (1) and (2), respectively, are absolutely continuous with respect to one another[23] and

$$\mu_T(B) = \int_B \rho(x)\mu_W(dx) \tag{3}$$

on any Borel set B. The density of the probability measure μ_T with respect to μ_W is $\rho(x) = (d\mu_T/d\mu_W)(x)$. A knowledge of ρ, as a functional of the sample paths of the process $\{X(t), t_0 \leqslant t \leqslant t_1\}$ enables us to evaluate the probabilities of various events of the biased Brownian motion $\tilde{X}(t)$ in terms of the unbiased diffusion process $X(t)$.

The transformation of diffusion processes, through the application of a nonequilibrium thermodynamic constraint which is then suddenly released, allows us to formulate a general principle of irreversible thermodynamics: In the near equilibrium regime, the fractional increment in the relative distribution of the density of paths of a biased diffusion process with respect to the unbiased process is equal to one-half of the product of the thermodynamic force and the increment of the unbiased diffusion process. This is expressed mathematically as

$$d\rho/\rho = \tfrac{1}{2}\chi(X(t))dX(t). \tag{4}$$

The factor of one-half is dictated by equilibrium statistical thermodynamics, which is obtained in the asymptotic time limit (cf. Sec. III).

Physically speaking, the thermodynamic principle (4) implicates the thermodynamic force as the cause of the incremental change in the relative probability density of paths belonging to the biased diffusion process with respect to the unbiased diffusion process. Moreover, this principle leads to a generalization of Boltzmann's principle for an irreversible thermodynamic process [cf. Eq. (25)].

The generalization to thermodynamic irreversible processes occurring in far from equilibrium regimes is purely formal. Since a nonequilibrium stationary state is maintained by a finite, external constraint, it is necessary to consider the transformation of one biased diffusion process into another one with the same diffusion coefficient but with a different thermodynamic force. In place of (4), we now have

$$d\rho/\rho = \tfrac{1}{2}\Delta\chi(X(t))dX(t), \tag{4'}$$

where $\Delta\chi$ is the difference in the thermodynamic forces of the two diffusion processes. In other words, (4') considers two relaxation processes with different driving forces that evolve to different, asymptotic stationary states. Both states cannot correspond to thermodynamic equilibrium since this state is uniquely determined by the principle of microscopic reversibility. Hereafter we shall restrict our discussion to the thermodynamic principle (4) since its generalization (4') follows straightforwardly.

Assume that the thermodynamic force of the biased diffusion process (2) is a gradient, viz.,

$$\chi(x) = \partial_x S(x), \tag{5}$$

where S is the entropy of the nonequilibrium state x. From classical considerations, we would expect the gradient condition to imply that the integral of (4) be equal to the difference in entropies of the given nonequilibrium states. This, however, is not the case since the two nonequilibrium states are statistically correlated and consequently the transition between two nonequilibrium states cannot be related simply to the difference in a thermodynamic function of state. In other words, the existence of statistical correlations between nonequilibrium states destroys the thermodynamic additive property of $\ln\rho$ and it follows that $d\ln\rho \neq d\rho/\rho$.

In order to take into consideration the statistical correlations that exist between nonequilibrium states which are not well separated in time, it is necessary to use stochastic rather than ordinary calculus. According to the Itô chain rule of stochastic calculus[24] we have that

$$d\ln\rho = d\rho/\rho - \tfrac{1}{2}(d\rho/\rho)^2 \tag{6}$$

which, on account of the Brownian motion phenomenon

$$E\{dX^2(t)\} = \sigma^2\, dt \tag{7}$$

tends, in probability, to

$$d\ln\rho = \tfrac{1}{2}\{\chi(X(t))dX(t) - \tfrac{1}{4}\sigma^2\chi^2(X(t))dt\}. \tag{8}$$

In expression (7), E denotes the mathematical expectation. Then integrating over the time interval $[t_0,t_1]$ we obtain

$$\ln\rho(X(t)) = \tfrac{1}{2}\int_{t_0}^{t_1}\{\chi(X(t))dX(t) - \tfrac{1}{4}\sigma^2\chi^2(X(t))dt\}. \tag{9}$$

Expression (9) is in a somewhat inconvenient form due to the presence of the stochastic integral. The stochastic integral can be eliminated by taking into account Itô's formula

$$\int_{t_0}^{t_1}\chi(X(t))dX(t) = S(X(t_1)) - S(X(t_0)) - \tfrac{1}{2}\sigma^2\int_{t_0}^{t_1}\partial_x\chi(X(t))dt. \tag{10}$$

Equation (10) defines the "stochastic" entropy which is a functional of the process $X(t)$. Eliminating the stochastic integral between Eqs. (9) and (10), we get

$$\ln\rho(X(t)) = \tfrac{1}{2}\{S(X(t_1)) - S(X(t_0)) - \int_{t_0}^{t_1}V(X(t))dt\}, \tag{11}$$

where V is the so-called Onsager–Machlup potential[16]

$$V(x) = L\{\tfrac{1}{2}\chi^2(x) + \partial_x\chi(x)\}. \tag{12}$$

The time integral in expression (11) describes the statistical correlations between the endpoints of the transition. It is responsible for the destruction of the thermodynamic additivity property of $\ln\rho$ and it makes it a path dependent quantity; that is, it is a functional of the sample paths of the process $X(t)$.

III. THERMODYNAMICS OF STATISTICALLY CORRELATED NONEQUILIBRIUM STATES

Using the results of the previous section, we derive the formula for the transition density function of the irreversible thermodynamic process $\tilde{X}(t)$ in terms of the process $X(t)$. Since the process is Markov, this together with the probability density function gives a complete statistical description of the process. This is to say that any joint probability density can be constructed by taking products of the transition probability density which are multiplied by the probability density for the initial state. The latter is known from the entropy function by Boltzmann's principle.

It is a peculiarity of diffusion processes that the transition density is completely determined by the first two moments of a conditional distribution.[25] In general, a distribution is not determined by two of its moments unless it happens to be Gaussian. This is the key point in generalizing the Onsager–Machlup formulation[2] to non-Gaussian, diffusion processes.

Let $\tilde{X}_{x_0,t_0}(t)$ be the solution of the stochastic differential equation (2) for $t > t_0$ with initial condition $\tilde{X}_{x_0,t_0}(t_0) = x_0$. The transition probability $P_T(B,t_1|x_0,t_0)$ will coincide with the probability $\mathscr{P}\{\tilde{X}_{x_0,t_0}(t_1)\in B\}$ and

$$P_T(B,t_1|x_0,t_0) = \mathscr{P}\{\tilde{X}_{x_0,t_0}(t_1)\in B\} = \mu_T(B). \tag{13}$$

Then in view of expression (3), we have

$$P_T(B,t_1|x_0,t_0) = \int_B E\{\rho(X(t))|X_{x_0,t_0}(t_1)\} \times p_W(x,t_1|x_0,t_0)dx, \tag{14}$$

where $E\{\cdot|X_{x_0,t_0}(t_1)\}$ denotes the conditional expectation with respect to the final point of the transition and X_{x_0,t_0} is the solution of the stochastic differential equation (1) with

initial condition $X_{x_0,t_0}(t_0) = x_0$.

In Eq. (14), p_W denotes the transition probability density of the Wiener process,

$$p_W(x,t_1|x_0,t_0) = \{2\pi\sigma^2(t_1 - t_0)\}^{-1/2} \times \exp\{-(x - x_0)^2/2\sigma^2(t_1 - t_0)\}. \quad (15)$$

Equation (14) shows that there exists a density $p_T(x,t_1|x_0,t_0)$ corresponding to the transition probability

$$P_T(B,t_1|x_0,t_0) = \int_B p_T(x,t_1|x_0,t_0)dx, \quad (16)$$

where

$$p_T(x,t_1|x_0,t_0) = E\{\rho(X(t))|X_{x_0,t_0}(t_1)\}p_W(x,t_1|x_0,t_0). \quad (17)$$

Relation (17) is a fundamental result: The transition densities of the biased and unbiased diffusion processes are related by the conditional expectation of the relative probability density of the paths of the biased diffusion process with respect to the probability density of paths of the unbiased diffusion process. This path average, between fixed endpoints of the transition, transforms the transition density of the unbiased Brownian motion into the transition density for the biased Brownian motion which is our irreversible thermodynamic process. We now cast this path average into a more suggestive form.

Introducing the expression for ρ, given in (11), into (17) yields

$$p_T(x,t_1|x_0,t_0) = \exp\{\tfrac{1}{2}[S(x) - S(x_0)]\}\cdot K(x,t_1|x_0,t_0), \quad (18)$$

where the transformation function or kernel K is given by

$$K(x,t_1|x_0,t_0) = E\left\{\exp\left[-\tfrac{1}{2}\int_{t_0}^{t_1} V(X(t))dt\right]\middle| X_{x_0,t_0}(t_1)\right\} \times p_W(x,t_1|x_0,t_0). \quad (19)$$

It will now be appreciated that (19) is the Feynman–Kac formula that expresses the kernel as a conditional Wiener integral for the potential $V(x)$[26]. It is a well-known result that the evaluation of the conditional Wiener integral (19) can be reduced to solving the diffusion equation

$$\partial_{t_1} K = L\partial_x^2 K - \tfrac{1}{2}V(x)K, \quad (20)$$

which is closely allied with Schrödinger's equation. In order that (19) represent a physically acceptable solution of Eq. (20), certain restrictions must be placed on the potential V. It will be shown elsewhere[17] that these restrictions are related to the stochastic stability of the process.

We have previously remarked that the time integral of the Onsager–Machlup potential (12) describes the statistical correlations between nonequilibrium states. This information is likewise contained in the kernel (19). A quasithermodynamic quantity can be associated with the logarithm of the kernel in an analogous way so that Boltzmann's principle relates the entropy to the probability density in the asymptotic time limit, viz.,

$$\ln p_\infty(x) = S(x) + \text{const}, \quad (21)$$

where

$$\lim_{\tau\to\infty} p_T(x,\tau|x_0) = p_\infty(x). \quad (22)$$

The change in notation $\tau = t_1 - t_0$, emphasizes the stationarity of the process in the wide sense. Expression (22) states that in "aged" (stable) systems (i.e., those in which the statistical correlations between nonequilibrium states have had ample time to wear off), the transition density transforms into the limiting stationary distribution. In view of (18), this means that

$$\lim_{\tau\to\infty} \ln K(x,\tau|x_0) = \tfrac{1}{2}\{S(x) + S(x_0)\} + \text{const}. \quad (23)$$

It now becomes apparent why the factor of one-half appears in the thermodynamic principle (4): It provides the correct limiting statistical distribution in the asymptotic time limit.

The fact that the logarithm of the kernel is related to the sum of entropies in the asymptotic time limit implies that the two nonequilibrium states are statistically independent. If, however, a sufficient amount of time has not elapsed, the nonequilibrium states will be correlated statistically and $\ln K$ will not reduce to a sum of entropies, as in (23). This fact motivates the definition

$$\ln K(x,\tau|x_0) = \tfrac{1}{2}\sigma_J(x,\tau;x_0) \quad (24)$$

of the joint entropy σ_J. The properties of the joint entropy provide a detailed description of the statistical correlations between nonequilibrium states. Because it is a function of the endpoints of transition as well as the time interval of transition, the joint entropy must be considered as a quasithermodynamic quantity.

Taking the logarithm of (18) and using (24), we obtain the kinetic analog of Boltzmann's principle (21), viz.,

$$\ln p_T(x,\tau|x_0) = \tfrac{1}{2}\{S(x) - S(x_0) + \sigma_J(x,\tau;x_0)\}. \quad (25)$$

In view of the asymptotic limit (22), it is necessary that

$$\lim_{\tau\to\infty} \sigma_J(x,\tau;x_0) = S(x) + S(x_0) + \text{const}. \quad (26)$$

The proof that (26) is the correct asymptotic limit entails solving the diffusion equation (20) for the asymptotic stationary solution. However, it is easier to use the logarithmic transformation (24) and solve the generalized Hamilton–Jacobi equation

$$-\partial_\tau\sigma_J + \tfrac{1}{2}L(\partial_x\sigma_J)^2 + L\partial_x^2\sigma_J = V(x) \quad (27)$$

in the asymptotic time limit. The stationary solution ($\partial_\tau\sigma_J = 0$) can be gleaned from the Onsager–Machlup potential (12); after integration we obtain

$$\sigma_J(x,\tau = \infty;x_0) = S(x) + C(x_0). \quad (28)$$

The constant of integration, C, can be determined by considering the stationary solution of the "backward" diffusion equation (replacing t_1 by $-t_0$ and x by x_0) for the kernel

$$\partial_\tau K = L\partial_{x_0}^2 K - \tfrac{1}{2}V(x_0)K. \quad (29)$$

Equivalently, we can consider the stationary solution of the "backward" Hamilton–Jacobi equation

$$-\partial_\tau\sigma_J + \tfrac{1}{2}L(\partial_{x_0}\sigma_J)^2 + L\partial_{x_0}^2\sigma_J = V(x_0). \quad (30)$$

Now in order that the stationary solution of Eq. (30) be compatible with the stationary solution (28), it is necessary to set the constant of integration $C(x_0) = S(x_0) + \text{const}$. This then establishes the validity of the asymptotic limit in (26).

Furthermore, an additional quasithermodynamic quantity can be defined according to

$$\sigma_C(x,\tau|x_0) = \sigma_J(x,\tau;x_0) - S(x_0), \tag{31}$$

which is the conditional entropy. In the asymptotic time limit, it transforms into the entropy of the given nonequilibrium state. This is easily demonstrated by taking the asymptotic time limit in (31) and using (26). We then obtain

$$\lim_{\tau\to\infty} \sigma_C(x,\tau|x_0) = S(x) + \text{const.} \tag{32}$$

Qualitatively speaking, (32) expresses the fact that a dissipative system forgets its past.

IV. GROWTH AND DECAY OF FLUCTUATIONS

In this section, the close analogy between the forward diffusion equation (20) and Schrödinger's equation will be used to investigate the growth and decay of fluctuations in nonequilibrium thermodynamic processes. The important result of the analysis will be to show that the macroscopic, phenomenological laws of irreversible thermodynamics emerge in the exact balance between the rates of growth and decay of fluctuations. This generalizes previous results that are strictly valid for Gaussian diffusion processes which display a symmetry in past and future.[2,19] For Gaussian fluctuations, the "smoothest" path is a superposition of decaying and growing exponentials in time.

It is a well-known property that if $V(x)\to\infty$ as $x\to\pm\infty$ the eigenvalue problem

$$L\partial_x^2\phi - \tfrac{1}{2}V(x)\phi = -\gamma\phi \tag{33}$$

yields a discrete spectrum of eigenvalues $\gamma_0,\gamma_1,\gamma_2,\ldots$ with the corresponding normalized eigenfunctions $\phi_0,\phi_1,\phi_2,\ldots$. The problem is then of the Sturm–Liouville type in which all eigenvalues are real and the sequence of eigenvalues forms an infinitely denumerable sequence that can be ordered in such a way that $\gamma_{n+1} > \gamma_n$, $n = 0,1,2,\ldots$. One advantage of considering Eq. (33) instead of the diffusion equation (20) is that the time factor $e^{-\gamma\tau}$ has been split off. In fact, the kernel can be expressed as a bilinear sum of normalized eigenfunctions with each term being weighted by the appropriate exponential time factor, viz.,[27]

$$K(x,\tau|x_0) = \sum_{n=0}^{\infty} \phi_n(x)\phi_n(x_0)e^{-\gamma_n\tau}. \tag{34}$$

We have thus succeeded in expressing an integral over a space of functions, (19), as a purely classical quantity in (34).

The "ground state" eigenfunction, which is related to the asymptotic stationary distribution, can be found by considering (12) as an equation for the thermodynamic force rather than the definition of the Onsager–Machlup potential. Let $\chi = \partial_x \ln\psi^2$, say, and introduce it into Eq. (12). We then obtain

$$L\partial_x^2\psi - \tfrac{1}{2}V(x)\psi = 0. \tag{35}$$

On comparing Eq. (33) with Eq. (35), we identify $\psi\equiv\phi_0$, the ground state eigenfunction with eigenvalue $\gamma_0 = 0$.

Parenthetically, we remark that the stochastic correction term in the Onsager–Machlup potential (12) plays a fundamental role in setting up the limiting stationary distribution. In its absence, we would obtain a nonzero ground state eigenvalue, comparable to the zero-point energy of the harmonic oscillator. As a consequence, the eigenfunction expansion of the transition density [cf. Eq. (38)] would contain an exponential decaying factor in time in the principal term of this expansion. Hence, there would be no stationary statistical distribution to which the transition probability density would approach in the asymptotic time limit. Therefore, the stochastic correction term, which describes the random fluctuations, is essential to the establishment of the stationary statistical distribution. In general, these random fluctuations work against the stability of irreversible thermodynamic processes but they are nevertheless the essential factor which establishes the stationary statistical distribution.[15]

Returning to the discussion of the ground state eigenfunction, it now follows from the definition of the thermodynamic force, (5), that

$$\ln\phi_0^2(x) = S(x) + \text{const.} \tag{36}$$

On comparison with Boltzmann's principle (21), we obtain $p_\infty(x) = \phi_0^2(x)$. We have thus defined the stationary statistical distribution in terms of the ground state eigenfunction as well as the thermodynamic force

$$\chi(x) = 2\partial_x \ln\phi_0(x). \tag{37}$$

This is to say that the thermodynamic force is defined *solely* in terms of the stationary statistical distribution, or equivalently, in terms of the ground state eigenfunction.

On the strength of expressions (34) and (36), the transition density (18) can be written as the eigenfunction series expansion

$$p_T(x,\tau|x_0) = \phi_0^2(x) + \phi_0(x)/\phi_0(x_0) \times \sum_{n=1}^{\infty} \phi_n(x)\phi_n(x_0)e^{-\gamma_n\tau}. \tag{38}$$

It is easy to see that (38) is the solution to the forward Fokker–Planck equation

$$\partial_\tau p_T(x,\tau|x_0) = -\partial_x j(x,\tau|x_0), \tag{39}$$

with an initial distribution given by

$$p_T(x,\tau|x_0) = \delta(x - x_0) \quad \text{as } \tau\to 0.$$

The forward Fokker–Planck equation (39) has been written in the form of a continuity equation, where the transition probability flux density j is given by

$$j = L\{p_T\partial_x S - \partial_x p_T\}, \tag{40}$$

or in terms of the eigenfunction series expansion

$$j = L\sum_{n=1}^{\infty} \frac{\phi_n(x_0)}{\phi_0(x_0)} \times \{\phi_n(x)\partial_x\phi_0(x) - \phi_0(x)\partial_x\phi_n(x)\}e^{-\gamma_n\tau}. \tag{41}$$

The transition probability flux density describes transitions between excited (nonequilibrium) states and the ground (equilibrium) state.

In view of (36), the transition density can be written in the form

$$p_T(x,\tau|x_0) = \phi_0(x)K(x,\tau|x_0)\phi_0^{-1}(x_0). \tag{42}$$

Introducing (42) into (41) and using definition (24) results in (24) results in

$$j(x,\tau|x_0) = \tfrac{1}{2}Lp_T\{\partial_x S - \partial_x\sigma_J\}, \tag{43}$$

which has a form similar to that of a macroscopic, phenomenological force-flux relation

$$J = L\partial_x S. \tag{44}$$

J is the thermodynamic flux and Eq. (44) is the average of the stochastic differential equation (2) in accordance with Onsager's regression hypothesis.[1,2] The relationship between (43) and (44) can be preceived if we define

$$J(x) = v(x,\tau|x_0) + u(x,\tau|x_0)$$

and

$$j(x,\tau|x_0) = p_T(x,\tau|x_0)v(x,\tau|x_0). \tag{45}$$

It then follows that

$$v(x,\tau|x_0) = \tfrac{1}{2}L\{\partial_x S(x) - \partial_x \sigma_J(x,\tau;x_0)\}, \tag{46}$$

$$u(x,\tau|x_0) = \tfrac{1}{2}L\{\partial_x S(x) + \partial_x \sigma_J(x,\tau;x_0)\}. \tag{47}$$

The separation of the thermodynamic flux J into two transitional velocities v and u decomposes the motion into the rates of growth and decay of fluctuations back to equilibrium, respectively.

The two transitional velocities are mirror images of one another (τ replacing $-\tau$). This is a general characteristic that applies to all stationary diffusion processes; it is a consequence of the fact that the joint entropy is an odd function of the time interval τ. The transitional velocities are functions of both endpoints of transition as well as the time interval. The surprising fact is that their sum, the thermodynamic flux, is a function of the present state of the system. This has been achieved by an exact balance between the rates of growth and decay of fluctuations. In other words, on account of the time-inversion symmetry, all information regarding the initial state has no influence on the macroscopic evolution of irreversible thermodynamic processes. This applies to non-Gaussian as well as Gaussian diffusion processes and generalizes our previous results.[19] We shall now illustrate these results by taking the particular case of the Ornstein–Uhlenbeck process in configuration space.

If we expand the entropy in a Taylor series about equilibrium, we have

$$S(x) = S_0 - \tfrac{1}{2}Q_\infty^{-1}x^2 + \text{higher terms}, \tag{48}$$

where Q_∞ is the equilibrium second moment. Neglect of the higher terms means that we are making the Gaussian assumption. In view of the definition of the thermodynamic force, (5), we have

$$\chi = -Q_\infty^{-1}x \tag{49}$$

which, in the Gaussian approximation, is a linear restoring force. The Onsager–Machlup potential (12), for the Gaussian diffusion process, is

$$V = L\{\tfrac{1}{2}Q_\infty^{-2}x^2 - Q_\infty^{-1}\}. \tag{50}$$

With the Onsager–Machlup potential (50), the conditional Wiener integral (19) for the kernel can be evaluated. The path average yields an explicit expression for the kernel, since the integrals are Gaussian, in terms of the endpoints of the transition and the time interval for the transition. However, a more physically intuitive method can be used that is based on the equality of means and modes of a Gaussian process. In this way, the origins of the stochastic correction terms can be clearly delineated.

The exponent in the conditional Wiener integral (19) can be written in the form of a thermodynamic action[6,27]

$$\mathscr{A}(x,\tau;x_0) = \int_0^\tau \mathscr{L}(x,\dot{x})dt = \tfrac{1}{2}\int_0^\tau L^{-1}\{\dot{x}^2 + V(x)\}dt. \tag{51}$$

On the strength of the identity between means and modes, a path average is equivalent to the requirement that the thermodynamic action be an extremum. The Euler–Lagrange equation for the extreme value of the integral is

$$d_t\partial_{\dot{x}}\mathscr{L} - \partial_x\mathscr{L} = 0 \tag{52}$$

or

$$\ddot{x} - \gamma^2 x = 0, \tag{53}$$

where $\gamma = LQ_\infty^{-1}$. The general solution to Eq. (53) is

$$x(\tau) = x_0\cosh\gamma\tau + (\dot{x}_0/\gamma)\sinh\gamma\tau, \tag{54}$$

where x_0 and $\dot{x}_0$ are the initial position and velocity, respectively. Introducing (54) into (51) and integrating yields

$$\mathscr{A}(x,\tau;x_0) = \tfrac{1}{2}Q_\infty^{-1}\{(x^2 + x_0^2)\cosh\gamma\tau - 2xx_0\}/\sinh\gamma\tau - \gamma\tau. \tag{55}$$

The thermodynamic action (55) differs from its deterministic counterpart by the last term in (55), which is the stochastic correction term that makes the stochastic integral (10) a martingale. Moreover, we cannot simply relate the thermodynamic action (55) to the kernel since there is an inherent indeterminancy in simultaneous position and velocity measurements. Analogous to the Heisenberg uncertainty principle of quantum mechanics, we cannot determine simultaneously, to any arbitrary degree of precision, both the velocity and position of the Brownian particle.[28] Hence, it is necessary to express the kernel as the stochastic integral

$$K(x,\tau|x_0) = \text{const}\exp\left\{-\frac{1}{2}\int_0^\tau d\mathscr{A}(x,t;x_0)\right\} = \text{const}\{Q(\tau)\}^{-1/2}\exp\{-\tfrac{1}{2}\mathscr{A}(x,\tau;x_0)\}, \tag{56}$$

since by the Itô chain rule

$$\begin{aligned} d\mathscr{A}(x,\tau;x_0) &= Q_\infty^{-1}\{(x\cosh\gamma\tau - x_0)/\sinh\gamma\tau\}dx \\ &\quad - \tfrac{1}{2}\gamma Q_\infty^{-1}\{(x^2 + x_0^2 - 2xx_0\cosh\gamma\tau)/\sinh^2\gamma\tau\}d\tau \\ &\quad + \gamma\coth\gamma\tau d\tau - \gamma d\tau. \end{aligned} \tag{57}$$

Moreover, since a precise knowledge of the endpoints of transition is equivalent to knowing the initial position and velocity of the Brownian particle, to any arbitrary degree of precision, allowance has been made for the uncertainty in the final endpoint in (57).[29] The last two terms in (57) are the stochastic correction terms which, when integrated over the time interval, determine the correct normalizing factor for the kernel, viz.,

$$\gamma\int_0^\tau(\coth\gamma t - 1)dt = \ln(\sinh\gamma\tau/e^{\gamma\tau}) = \ln\{\tfrac{1}{2}(1 - e^{-2\gamma\tau})\}. \tag{58}$$

Thus, the kernel is given explicitly as

$$K(x,\tau|x_0) = \{4\pi Q_\infty \sinh \gamma\tau/e^{\gamma\tau}\}^{-1/2} \times \exp\{-((x^2 + x_0^2)\cosh \gamma\tau - 2xx_0)/4Q_\infty \sinh \gamma\tau\}, \tag{59}$$

and from expression (18) we obtain the transition density,

$$p_T(x,\tau|x_0) = \{2\pi Q_\infty(1 - e^{-2\gamma\tau})\}^{-1/2} \times \exp\{-(x - x_0e^{-\gamma\tau})^2/2Q_\infty(1 - e^{-2\gamma\tau})\}. \tag{60}$$

Expression (60) is a well-known result; the reason for its detailed derivation was to display the stochastic origins of the normalization factor. In fact, its time rate of change is related to the compressibility of fluid motion of the volume occupied by the path trajectories in configuration space.

The space derivative of the joint entropy is

$$\partial_x \sigma_J = 2\partial_x \ln K = -Q_\infty^{-1}(x\cosh \gamma\tau - x_0)/\sinh \gamma\tau. \tag{61}$$

Introducing expressions (49) and (61) for the two forces into the transitional velocity expressions (46) and (47), we obtain

$$v = -LQ^{-1}(-\tau)(x - x_0e^{\gamma\tau}) \tag{62}$$

and

$$u = -LQ^{-1}(\tau)(x - x_0e^{-\gamma\tau}), \tag{63}$$

where $Q(\tau)$ is the second moment of the distribution,

$$Q(\tau) = Q_\infty(1 - e^{-2\gamma\tau}), \tag{64}$$

and $Q(-\tau)$ is its mirror image in time ($-\tau$ replacing τ). It will also be appreciated that the transitional velocities, (62) and (63), are mirror images of one another in time. The transitional velocity v is the rate of growth of fluctuations from the most probable path for their growth, along which it vanishes. Likewise, the transitional velocity u is the rate of decay of fluctuations from the most probable path for their decay to equilibrium. Along this path, u vanishes. On the average, these two effects balance one another and what is observed macroscopically is the thermodynamic flux J, the sum of the two transitional velocities.

The thermodynamic force is the driving force toward equilibrium; it is a measure of the attraction of the equilibrium state. On the other hand, the gradient of the joint entropy is a measure of the strength of statistical correlations between nonequilibrium states. In the asymptotic time limit, the statistical correlations have worn off and we have

$$\lim_{\tau\to\infty} \partial_x \sigma_J(x,\tau;x_0) = \chi(x). \tag{65}$$

The system has decayed back to equilibrium where only spontaneous fluctuations occur. The transitional velocity v vanishes and u coincides with the thermodynamic flux J. We emphasize that our stochastic analysis provides for the correct limiting statistical distribution in which the x are spontaneous fluctuations from equilibrium that obey the phenomenological relations (44). This is to say, that as far as the average behavior is concerned, it does not matter whether a state was the result of a spontaneous fluctuation or of an imposed constraint. For non-Gaussian fluctuations, these results remain valid with the exception that the transitional velocities will not vanish on the most probable path for the growth or decay of a fluctuation. They are then related to the average, rather than the most probable, behavior of the course of a fluctuation.

The transitional velocity for the growth of fluctuations is involved in the establishment of the asymptotic statistical distribution. Its nonvanishing space derivative,

$$d_\tau p_T = -p_T\partial_x v, \tag{66}$$

allows us to draw the analogy with compressible fluid motion. This compressible fluid motion is related to the rate at which the distribution spreads in time. In the case of the Ornstein–Uhlenbeck process, we have

$$-\partial_x v = \gamma(1 - e^{2\gamma\tau})^{-1} = \tfrac{1}{2}d_\tau \ln Q(\tau), \tag{67}$$

where expression (62) has been substituted into (66). In other words, the stochastic uncertainty of the process is responsible for the variation in the volume occupied by the path trajectories. Although we have shown this result only in the particular case of Gaussian diffusion processes, we expect that it should be valid in the general case since the transition densities of diffusion processes are determined completely by the first two moments.[25]

Turning to the transitional velocity for the rate of decay of fluctuations, we see that in order for (45) to be compatible with (40), u must satisfy the condition

$$u(x,\tau|x_0) = L\partial_x \ln p_T(x,\tau|x_0), \tag{68}$$

which is another way of expressing (47). On account of the statistical correlations between nonequilibrium states, the transitional velocity for the rate of decay of fluctuations cannot be derived from a velocity potential. In general, no potential conditions can be imposed on the velocity u because the transition density cannot be determined in terms of a difference in a thermodynamic function of state. Therefore, the transitional velocity will be a nonlocal function with an explicit dependence on the time interval of transition. Results, contrary to ours, have appeared in the literature.[20]

However, in the asymptotic time limit where the transition density transforms into the stationary probability density (22), we have

$$\lim_{\tau\to\infty} u(x,\tau|x_0) = L\partial_x \ln p_\infty(x). \tag{69}$$

Relation (69) is none other than the Einstein criterion for dynamic equilibrium in a suspension of Brownian particles. In a state of dynamic equilibrium, the osmotic pressure force $\partial_x \ln p_\infty$ is balanced by the (fluctuating) velocity acquired by a Brownian particle due to the action of a (virtual) external force.

Relation (69), together with Boltzmann's principle (21), give

$$\lim_{\tau\to\infty} u(x,\tau|x_0) = L\partial_x S(x), \tag{70}$$

thus showing that the entropy is the velocity potential for the (fluctuating) velocity u in the asymptotic time limit. The interesting conclusion that can be drawn is that the behavior of the decay of a spontaneous fluctuation back to equilibrium depends solely on the nonequilibrium state in which it is found. This confirms and generalizes our previous results.[19,28] Out of a state of dynamic equilibrium, no potential condition can be imposed on the transitional velocity for the

decay of fluctuations due to the presence of statistical correlations that make the transition density dependent on the endpoints of transition as well as the time interval transition.

ACKNOWLEDGMENT

We acknowledge the Ministero della Pubblica Istruzione for financial assistance.

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The uniqueness of gravity as a Poincaré or Lorentz gauge theory

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(Received 27 February 1980; accepted for publication 7 August 1980)

The uniqueness of the Einstein–Cartan–Sciama–Kibble theory is examined using a concomitant approach. The demand that the Lagrangian be a scalar density under coordinate transformations and a scalar under Poincaré or Lorentz gauge transformations as well as be degenerate in the order of the Euler–Lagrange expressions determines a class of Lagrangians whose Euler–Lagrange equations reduce essentially to the Einstein vacuum field equations with cosmological term.

PACS numbers: 11.10.Np, 11.30.Cp, 04.20.Fy

1. INTRODUCTION

Several attempts[1] have been made to show that the Einstein–Cartan–Sciama–Kibble theory[2] is, in some sense, a unique theory for the Poincaré group. Rigorous mathematical techniques have not been applied and their use of the term gauge theory is somewhat questionable since their so-called gauge transformations are induced by coordinate transformations based on the Poincaré group.

In this paper we shall use the local formalism developed previously[3] and so we shall restrict ourselves to the connected component of the identity of the Poincaré group. At each point of the space–time manifold M (local coordinates x^i, $i = 1,...,4$), we associate a group element $u = u(x^i)$. We shall be concerned with two kinds of transformations: coordinate transformations, denoted by a horizontal bar, and Poincaré gauge transformations, denoted by a prime. A coordinate transformation

$$\bar{x}^i = \bar{x}^i(x^j),$$

is characterized by

$$J^i_{\ j} \equiv \partial x^i/\partial \bar{x}^j,$$

with

$$J \equiv \det J^i_{\ j} \neq 0.$$

By a Poincaré gauge transformation we shall mean a 10-parameter transformation where the parameters $u^{\alpha\beta}(x^i) = -u^{\beta\alpha}(x^i)$ and $u^\alpha(x^i)$, $\alpha, \beta = 1,...,4$, are the coordinates of $u(x^i)$ relative to a canonical chart of the first kind.[4] Under a Poincaré gauge transformation the local coordinates of M are invariant, i.e.,

$$x'^i = x^i$$

while, for example, an orthonormal tetrad (or vierbein) $h^{\ \alpha}_i$ undergoes a Lorentz transformation, i.e.,

$$h'^{\ \alpha}_i = \mathscr{L}^\alpha_{\ \beta} h^{\ \beta}_i,$$

where

$$\mathscr{L}^\alpha_{\ \beta} \equiv \exp(-u^{\alpha\gamma}\eta_{\gamma\beta}),$$

with

$$\eta_{\gamma\beta} \equiv \mathrm{diag}(-1,-1,-1,1).$$

With every gauge theory there arise quantities known as gauge connections (or gauge potentials). For the Poincaré group these will be denoted by $A_i^{\ \alpha\beta} = -A_i^{\ \beta\alpha}$ and $A_i^{\ \alpha}$. The corresponding gauge curvatures are, by definition,

$$F_i^{\ \alpha\beta}{}_j \equiv A_{i,j}^{\ \alpha\beta} - A_{j,i}^{\ \alpha\beta} - C_{\mu\nu}^{\ \ \alpha\beta}{}_{\gamma\omega} A_i^{\ \mu\nu} A_j^{\ \gamma\omega} - C_\mu^{\ \alpha\beta}{}_{\gamma\omega} A_i^{\ \mu} A_j^{\ \gamma\omega} - C_{\mu\nu}^{\ \ \alpha\beta}{}_\gamma A_i^{\ \mu\nu} A_j^{\ \gamma} - C_\mu^{\ \alpha\beta}{}_\gamma A_i^{\ \mu} A_j^{\ \gamma},$$

and

$$F_i^{\ \alpha}{}_j \equiv A_{i,j}^{\ \alpha} - A_{j,i}^{\ \alpha} - C_{\mu\nu}^{\ \ \alpha}{}_{\gamma\omega} A_i^{\ \mu\nu} A_j^{\ \gamma\omega} - C_\mu^{\ \alpha}{}_{\gamma\omega} A_i^{\ \mu} A_j^{\ \gamma\omega} - C_{\mu\nu}^{\ \ \alpha}{}_\gamma A_i^{\ \mu\nu} A_j^{\ \gamma} - C_\mu^{\ \alpha}{}_\gamma A_i^{\ \mu} A_j^{\ \gamma},$$

where the $C_{\mu\nu}^{\ \ \alpha\beta}{}_{\gamma\omega}$, $C_\mu^{\ \alpha\beta}{}_{\gamma\omega}$,..., and $C_\mu^{\ \alpha}{}_\gamma$ are the structure constants of the Poincaré group.

Kibble[2] dealt with just the Lorentz group and the Lagrangian

$$L = h h^i_{\ \alpha} h^j_{\ \beta} F_i^{\ \alpha\beta}{}_j, \tag{1.1}$$

where

$$h \equiv |\det h^{\ \alpha}_i| \neq 0,$$

$h^j_{\ \beta}$ is the inverse of $h^{\ \alpha}_i$, i.e.,

$$h^j_{\ \alpha} h^{\ \alpha}_i = \delta^j_i,$$

and

$$h^i_{\ \beta} h^{\ \alpha}_i = \delta^\alpha_\beta,$$

and $F_i^{\ \alpha\beta}{}_j$ is the Lorentz gauge curvature given by

$$F_i^{\ \alpha\beta}{}_j \equiv A_{i,j}^{\ \alpha\beta} - A_{j,i}^{\ \alpha\beta} + \eta_{\rho\omega}(A_i^{\ \alpha\rho} A_j^{\ \beta\omega} - A_j^{\ \alpha\rho} A_i^{\ \beta\omega}).$$

The corresponding Euler–Lagrange equations, viz.,

$$E^k_{\ \sigma\tau} \equiv \frac{\partial L}{\partial A_k^{\ \sigma\tau}} - \frac{\partial}{\partial x^l}\left(\frac{\partial L}{\partial A_{k,l}^{\ \sigma\tau}}\right) = 0,$$

and

$$\mathscr{E}^k_{\ \sigma} \equiv \frac{\partial L}{\partial h^{\ \sigma}_k} = 0,$$

reduce to the Einstein vacuum field equations, i.e.,

$$R_{ij} = 0,$$

where R_{ij} is the Ricci tensor of the Christoffel symbol. It is interesting to note that the Lagrangian (1.1) is degenerate in the sense that while it is first order in the gauge connection, i.e.,

$$L = L(h^{\ \alpha}_i; A_i^{\ \alpha\beta}; A_{i,j}^{\ \alpha\beta}),$$

the Euler–Lagrange expression $E^k_{\ \sigma\tau}$ is also first order in $A_i^{\ \alpha\beta}$,

 0022-2488/81/122934-09$01.00

i.e.,

$$E^{k}_{\sigma\tau} = E^{k}_{\sigma\tau}(h^{\alpha}_{i};h^{\alpha}_{i,j};A^{\alpha\beta}_{i};A^{\alpha\beta}_{i,j}) .$$

One would expect $E^{k}_{\sigma\tau}$ to be second order in $A^{\alpha\beta}_{i}$. A similar degeneracy also arises in the standard approach to general relativity where the Lagrangian is second order in the metric

$$g_{ij} = h^{\alpha}_{i}h^{\beta}_{j}\eta_{\alpha\beta} ,$$

with

$$g \equiv |\det g_{ij}| = h^{2} \neq 0 .$$

The Euler–Lagrange expression

$$\mathscr{E}^{ij} \equiv \frac{\partial L}{\partial g_{ij}} - \frac{\partial}{\partial x^{k}}\left(\frac{\partial L}{\partial g_{ij,k}}\right) + \frac{\partial^{2}}{\partial x^{h}\partial x^{k}}\left(\frac{\partial L}{\partial g_{ij,kh}}\right),$$

for the usual Lagrangian, viz.,

$$L = \sqrt{g}R ,$$

where R is the curvature scalar, is just second order in g_{ij} and not fourth order. Much success[5] has been obtained in examining the uniqueness of various theories by demanding that the appropriate degeneracy hold.

In this paper we shall consider Lagrangians of the form

$$L = L(h^{\alpha}_{i};A^{\alpha\beta}_{i};A^{\alpha}_{i};A^{\alpha\beta}_{i,j};A^{\alpha}_{i,j}) ,$$

which are scalar densities under a coordinate transformation, i.e.,

$$\bar{L} = JL , \tag{1.2}$$

scalars under a Poincaré gauge transformation, i.e.,

$$\overset{\prime}{L} = L , \tag{1.3}$$

and are degenerate in the sense that the Euler–Lagrange expressions $E^{k}_{\sigma\tau}$ and E^{k}_{σ} are only first order in the gauge connections, i.e.,

$$E^{k}_{\sigma\tau} = E^{k}_{\sigma\tau}(h^{\alpha}_{i};h^{\alpha}_{i,j};A^{\alpha\beta}_{i};A^{\alpha}_{i};A^{\alpha\beta}_{i,j};A^{\alpha}_{i,j}) ,$$

and

$$E^{k}_{\sigma} = E^{k}_{\sigma}(h^{\alpha}_{i};h^{\alpha}_{i,j};A^{\alpha\beta}_{i};A^{\alpha}_{i};A^{\alpha\beta}_{i,j};A^{\alpha}_{i,j}) .$$

It will be shown that with these conditions L is restricted to being

$$L = a_{1}\epsilon^{ijkh}\epsilon_{\alpha\beta\gamma\omega}F_{i}^{\alpha\beta}{}_{j}F_{k}^{\gamma\omega}{}_{h} + a_{2}\epsilon^{ijkh}\eta_{\alpha\gamma}\eta_{\beta\omega}F_{i}^{\alpha\beta}{}_{j}F_{k}^{\gamma\omega}{}_{h} + b_{1}hh^{i}_{\mu}h^{j}_{\nu}\eta^{\mu\gamma}\eta^{\nu\omega}\epsilon_{\alpha\beta\gamma\omega}F_{i}^{\alpha\beta}{}_{j} + b_{2}hh^{i}_{\alpha}h^{j}_{\beta}F_{i}^{\alpha\beta}{}_{j} + ch ,$$

where ϵ^{ijkh} and $\epsilon_{\alpha\beta\gamma\omega}$ are four-dimensional Levi-Civita symbols and a_1, a_2, b_1, b_2, and c are arbitrary constants. Notice that there are no terms involving $F_{i}^{\alpha}{}_{j}$. It is a simple matter to show that the same Lagrangian is obtained if we are concerned with just the Lorentz group. In order to complete the discussion we find that the Euler–Lagrange equations corresponding to this Lagrangian reduce essentially to the Einstein vacuum field equations with cosmological term, i.e.,

$$b_{2}R_{ij} = \tfrac{1}{2}cg_{ij} ,$$

provided that b_1 and b_2 are not both zero.

2. PRELIMINARIES

The Poincaré group is the semidirect product of the Lorentz group with $\mathbf{R}^4$, i.e., the elements u and v of the Poincaré group consist of the ordered pairs $(a^{\alpha}_{\beta},a^{\alpha})$ and $(b^{\alpha}_{\beta},b^{\alpha})$ with multiplication, $w = uv$, defined by

$$(a^{\alpha}_{\beta},a^{\alpha})\cdot(b^{\beta}_{\gamma},b^{\beta}) = (a^{\alpha}_{\beta}b^{\beta}_{\gamma},a^{\alpha}_{\beta}b^{\beta} + a^{\alpha}).$$

To obtain the structure constants and the adjoint representation[3] we must set up a canonical chart of the first kind.[4] It can be shown[6] that such a chart is given by

$$a^{\alpha}_{\beta} = \exp(u^{\alpha\gamma}\eta_{\gamma\beta}) \equiv \hat{\mathscr{L}}^{\alpha}_{\beta} ,$$

and

$$a^{\alpha} = l^{\alpha}_{\beta}u^{\beta} ,$$

where

$$l^{\alpha}_{\beta} \equiv \delta^{\alpha}_{\beta} + \frac{1}{2!}u^{\alpha\gamma}\eta_{\gamma\beta} + \frac{1}{3!}u^{\alpha\gamma}\eta_{\gamma\omega}u^{\omega\nu}\eta_{\nu\beta} + \cdots .$$

This is arrived at by first finding a basis for the left invariant vector fields of the semidirect product of Gl(4,R) with $\mathbf{R}^4$ and then calculating their integral curves starting from the identity, thereby determining the exponential map. We then restrict this to the subgroup, the Poincaré group. It should be noted that a^{α}_{β} is the inverse of the Lorentz transformation matrix $\mathscr{L}^{\alpha}_{\beta}$. Also, since $\mathscr{L}^{\alpha}_{\beta}$ is a Lorentz matrix it leaves $\eta_{\alpha\beta}$ invariant, i.e.,

$$\mathscr{L}^{\alpha}_{\mu}\eta_{\alpha\beta}\mathscr{L}^{\beta}_{\nu} = \eta_{\mu\nu} ,$$

and thus the Poincaré gauge transformation law for $\eta_{\alpha\beta}$ can be expressed as either

$$\mathscr{L}^{\mu}_{\alpha}\mathscr{L}^{\nu}_{\beta}\,\overset{\prime}{\eta}_{\mu\nu} = \eta_{\alpha\beta} ,$$

or

$$\overset{\prime}{\eta}_{\alpha\beta} = \eta_{\alpha\beta} .$$

As shown in Ref. 3 the inverse of the adjoint representation is given by

$$T^{\alpha\beta}_{\gamma\omega}(u) \equiv \left.\frac{\partial w^{\alpha\beta}}{\partial v^{\gamma\omega}}\right|_{v=e} , \quad T^{\alpha\beta}_{\gamma}(u) \equiv \left.\frac{\partial w^{\alpha\beta}}{\partial v^{\gamma}}\right|_{v=e} ,$$

$$T^{\alpha}_{\gamma\omega}(u) \equiv \left.\frac{\partial w^{\alpha}}{\partial v^{\gamma\omega}}\right|_{v=e} , \text{and} \quad T^{\alpha}_{\gamma}(u) \equiv \left.\frac{\partial w^{\alpha}}{\partial v^{\gamma}}\right|_{v=e} ,$$

where $w^{\alpha\beta}$ and w^{α} are the coordinates of

$$w = u^{-1}vu .$$

We thus have

$$T^{\alpha\beta}_{\gamma\omega}(u) = \mathscr{L}^{\alpha}_{[\gamma}(u)\mathscr{L}^{\beta}_{\omega]}(u) , \quad T^{\alpha\beta}_{\gamma}(u) = 0 ,$$

$$T^{\alpha}_{\gamma\omega}(u) = \mathscr{L}^{\alpha}_{[\gamma}(u)\eta_{\omega]\beta}l^{\beta}_{\mu}(u)u^{\mu} , \quad \text{and} \quad T^{\alpha}_{\gamma}(u) = \mathscr{L}^{\alpha}_{\gamma}(u) ,$$

where square brackets around indices denotes antisymmetrization. Since the gauge curvatures transform by means of the inverse of the adjoint representation under a gauge transformation,[3] we have

$$\overset{\prime}{F}_{i}^{\alpha\beta}{}_{j} = \mathscr{L}^{\alpha}_{\gamma}\mathscr{L}^{\beta}_{\omega}F_{i}^{\gamma\omega}{}_{j} , \tag{2.1}$$

and

$$\overset{\prime}{F}_{i}^{\alpha}{}_{j} = \mathscr{L}^{\alpha}_{\gamma}\eta_{\omega\beta}l^{\beta}_{\mu}u^{\mu}F_{i}^{\gamma\omega}{}_{j} + \mathscr{L}^{\alpha}_{\gamma}F_{i}^{\gamma}{}_{j} . \tag{2.2}$$

Relative to our chosen chart, the structure constants

$$C_{\mu\nu}{}^{\alpha\beta}{}_{\gamma\omega} \equiv \frac{\partial T_{\mu\nu}^{\alpha\beta}(u)}{\partial u^{\gamma\omega}}\bigg|_{u=e}, \text{ etc.,}$$

are thus

$$C_{\mu\nu}{}^{\alpha\beta}{}_{\gamma\omega} = -\tfrac{1}{4}\eta_{\rho\tau}(\delta_{\mu\nu}^{\alpha\rho}\delta_{\gamma\omega}^{\beta\tau} - \delta_{\gamma\omega}^{\alpha\rho}\delta_{\mu\nu}^{\beta\tau}),$$
$$C_{\mu}{}^{\alpha\beta}{}_{\gamma\omega} = -C_{\gamma\omega}{}^{\alpha\beta}{}_{\mu} = 0,$$
$$C_{\mu}{}^{\alpha\beta}{}_{\gamma} = 0, \quad C_{\mu\nu}{}^{\alpha}{}_{\gamma\omega} = 0,$$
$$C_{\mu}{}^{\alpha}{}_{\gamma\omega} = -C_{\gamma\omega}{}^{\alpha}{}_{\mu} = -\tfrac{1}{2}\delta_{\gamma\omega}^{\alpha\tau}\eta_{\tau\mu},$$

and

$$C_{\mu}{}^{\alpha}{}_{\nu} = 0.$$

The gauge curvatures then reduce to

$$F_i{}^{\alpha\beta}{}_j = A_{ij}^{\alpha\beta} - A_{j,i}^{\alpha\beta} + \eta_{\gamma\omega}(A_i^{\alpha\gamma}A_j^{\beta\omega} - A_j^{\alpha\gamma}A_i^{\beta\omega}),$$

and

$$F_i{}^{\alpha}{}_j = A_{i,j}^{\alpha} - A_{j,i}^{\alpha} + \eta_{\gamma\omega}(A_i^{\gamma}A_j^{\alpha\omega} - A_j^{\gamma}A_i^{\alpha\omega}).$$

Note that $F_i{}^{\alpha\beta}{}_j$ is the same here as for the Lorentz group. We are now ready to demand that our Lagrangian be degenerate.

3. DEGENERACY

To simplify our calculations we shall use upper case Greek letters to represent all 10 gauge indices, so that, for example, $A_i^{\Sigma}, \Sigma = 1,\ldots,10$, signifies the ordered pair $(A_i^{\alpha\beta}, A_i^{\alpha})$. We now seek all Lagrangians

$$L = L(h_i^{\alpha}; A_i^{\Sigma}; A_{i,j}^{\Sigma}),$$

which satisfy the transformation laws (1.2) and (1.3) and which are degenerate in the sense that the Euler–Lagrange expression

$$E_{\Sigma}^{k} \equiv \frac{\partial L}{\partial A_k^{\Sigma}} - \frac{\partial}{\partial x^l}\left(\frac{\partial L}{\partial A_{k,l}^{\Sigma}}\right), \tag{3.1}$$

is independent of $A_{i,jh}^{\Lambda}$, i.e.,

$$\frac{\partial E_{\Sigma}^{k}}{\partial A_{i,jh}^{\Lambda}} \equiv 0. \tag{3.2}$$

Expansion of (3.1) yields

$$E_{\Sigma}^{k} = \frac{\partial L}{\partial A_k^{\Sigma}} - \frac{\partial^2 L}{\partial h_a^{\gamma}\partial A_{k,l}^{\Sigma}}h_{a,l}^{\gamma} - \frac{\partial^2 L}{\partial A_a^{\Omega}\partial A_{k,l}^{\Sigma}}A_{a,l}^{\Omega} - \frac{\partial^2 L}{\partial A_{a,b}^{\Omega}\partial A_{k,l}^{\Sigma}}A_{a,bl}^{\Omega}.$$

Hence, the condition (3.2) reduces to

$$\frac{\partial^2 L}{\partial A_{i,j}^{\Lambda}\partial A_{k,h}^{\Sigma}} = \frac{-\partial^2 L}{\partial A_{i,h}^{\Lambda}\partial A_{k,j}^{\Sigma}},$$

which, when combined with the invariance identity[7] corresponding to (4.5) in Ref. 3, viz.,

$$\frac{\partial L}{\partial A_{i,j}^{\Lambda}} = -\frac{\partial L}{\partial A_{j,i}^{\Lambda}},$$

yields that $\partial^2 L/\partial A_{i,j}^{\Lambda}\partial A_{k,h}^{\Sigma}$ is totally antisymmetric in its lower case Latin indices. Therefore,

$$\frac{\partial^3 L}{\partial A_{i,j}^{\Lambda}\partial A_{k,h}^{\Sigma}\partial A_{a,b}^{\Omega}} \equiv 0,$$

and hence

$$\frac{\partial^2 L}{\partial A_{i,j}^{\Lambda}\partial A_{k,h}^{\Sigma}} = \epsilon^{ijkh}L_{\Lambda\Sigma}, \tag{3.3}$$

where ϵ^{ijkh} is the four-dimensional Levi-Civita symbol and

$$L_{\Lambda\Sigma} = L_{\Lambda\Sigma}(h_i^{\alpha}; A_i^{\Omega}).$$

By virtue of the transformation laws of $L_{\Lambda\Sigma}$ inherited from $\partial^2 L/\partial A_{i,j}^{\Lambda}\partial A_{k,h}^{\Sigma}$ we obtain the invariance identity corresponding to (4.6) in Ref. 3, viz.,

$$\partial L_{\Lambda\Sigma}/\partial A_i^{\Omega} \equiv 0,$$

and thus

$$L_{\Lambda\Sigma} = L_{\Lambda\Sigma}(h_i^{\alpha}).$$

Integration of (3.3) with respect to $A_{k,h}^{\Sigma}$ then yields

$$\frac{\partial L}{\partial A_{i,j}^{\Lambda}} = \epsilon^{ijkh}L_{\Lambda\Sigma}A_{k,h}^{\Sigma} + \mathscr{L}_{\Lambda}^{ij}(h_k^{\alpha}; A_k^{\Omega}),$$

which can be expressed in the more useful form

$$\frac{\partial L}{\partial A_{i,j}^{\Lambda}} = \tfrac{1}{2}\epsilon^{ijkh}L_{\Lambda\Sigma}F_k{}^{\Sigma}{}_h + L_{\Lambda}^{ij}(h_k^{\alpha}; A_k^{\Omega}), \tag{3.4}$$

where L_{Λ}^{ij} now inherits the transformation laws of $\partial L/\partial A_{i,j}^{\Lambda}$. The invariance identity for L_{Λ}^{ij} corresponding to (4.6) in Ref. 3 demands that

$$L_{\Lambda}^{ij} = L_{\Lambda}^{ij}(h_k^{\alpha}).$$

When (3.4) is integrated with respect to $A_{i,j}^{\Lambda}$ it is found that L can be expressed as

$$L = \tfrac{1}{8}\epsilon^{ijkh}L_{\Lambda\Sigma}F_i{}^{\Lambda}{}_jF_k{}^{\Sigma}{}_h + \tfrac{1}{2}L_{\Lambda}^{ij}F_i{}^{\Lambda}{}_j + L_0(h_k^{\alpha}).$$

Upon absorbing the various constants and returning to lower case Greek indices, we have established the following theorem.

Theorem 3.1: A necessary condition for a Lagrangian of the form

$$L = L(h_i^{\alpha}; A_i^{\alpha\beta}; A_i^{\alpha}; A_{i,j}^{\alpha\beta}; A_{i,j}^{\alpha}),$$

which is a scalar density under a coordinate transformation and a scalar under a Poincaré gauge transformation to be degenerate in the sense that the Euler–Lagrange expressions $E_{\sigma\tau}^{k}$ and E_{σ}^{k} satisfy

$$E_{\sigma\tau}^{k} = E_{\sigma\tau}^{k}(h_i^{\alpha}; h_{i,j}^{\alpha}; A_i^{\alpha\beta}; A_i^{\alpha}; A_{i,j}^{\alpha\beta}; A_{i,j}^{\alpha}),$$

and

$$E_{\sigma}^{k} = E_{\sigma}^{k}(h_i^{\alpha}; h_{i,j}^{\alpha}; A_i^{\alpha\beta}; A_i^{\alpha}; A_{i,j}^{\alpha\beta}; A_{i,j}^{\alpha}),$$

is that L must be of the general form

$$L = \epsilon^{ijkh}L_{\alpha\beta\gamma\omega}F_i{}^{\alpha\beta}{}_jF_k{}^{\gamma\omega}{}_h + \epsilon^{ijkh}L_{\alpha\beta\gamma}F_i{}^{\alpha\beta}{}_jF_k{}^{\gamma}{}_h + \epsilon^{ijkh}L_{\alpha\beta}F_i{}^{\alpha}{}_jF_k{}^{\beta}{}_h + L_{\alpha\beta}^{ij}F_i{}^{\alpha\beta}{}_j + L_{\alpha}^{ij}F_i{}^{\alpha}{}_j + L_0,$$

where the quantities $L_{\alpha\beta\gamma\omega}$, $L_{\alpha\beta\gamma},\ldots,L_0$ depend on h_i^{α} alone, inherit their transformation laws from L and its derivatives and have the symmetry properties

$$L_{\alpha\beta\gamma\omega} = -L_{\beta\alpha\gamma\omega} = -L_{\alpha\beta\omega\gamma}, \quad L_{\gamma\omega\alpha\beta} = L_{\alpha\beta\gamma\omega},$$
$$L_{\beta\alpha\gamma} = -L_{\alpha\beta\gamma}, L_{\beta\alpha} = L_{\alpha\beta}, \quad L_{\alpha\beta}^{ij} = -L_{\beta\alpha}^{ij} = -L_{\alpha\beta}^{ji},$$
and $L_{\alpha}^{ji} = -L_{\alpha}^{ij}$.

Remark: The above argument can be extended to the case where any m-dimensional Lie group is used and h_i^{α} is

replaced by any quantity $\rho^A, A = 1,...,M$ (but not its derivatives), as long as the gauge transformation law for ρ^A is of the form

$$\rho'^A = T^A_B(u^\Sigma)\rho^B, \quad \Sigma = 1,...,m .$$

If the dimension of the base manifold is $n = 4$ and the Lagrangian

$$L = L(\rho^A; A_i^\Sigma; A_{i,j}^\Sigma),$$

is required to have the desired degeneracy then we must be able to express L as

$$L = \epsilon^{ijkh} L_{\Lambda\Sigma}(\rho^A) F_i^{\ \Lambda}{}_j F_k^{\ \Sigma}{}_h + L^{ij}_\Lambda(\rho^A) F_i^{\ \Lambda}{}_j + L_0(\rho^A) .$$

For the case we are concerned with, viz., the Poincaré group, we shall now determine the structure of $L_{\alpha\beta\gamma\omega}$, $L_{\alpha\beta\gamma},...,L_0$ by exploiting their symmetry properties and transformation laws. First, recall that

$$\bar{h}_i^{\ \alpha} = J_i^{\ j} h_j^{\ \alpha}, \quad h'^{\alpha}_i = \mathcal{L}^\alpha_\beta h_i^{\ \beta},$$

and

$$\left.\frac{\partial \mathcal{L}^\alpha_\beta}{\partial u^{\gamma\omega}}\right|_{u=e} = -\tfrac{1}{2}\delta^{\alpha\theta}_{\gamma\omega}\eta_{\theta\beta} .$$

Thus

$$\left.\frac{\partial \bar{h}_i^{\ \alpha}}{\partial J^a_b}\right|_{J^r_s=\delta^r_s} = \delta^b_i h_a^{\ \alpha}, \quad \left.\frac{\partial h'^{\alpha}_i}{\partial u^{\gamma\omega}}\right|_{u=e} = -\tfrac{1}{2}\delta^{\alpha\theta}_{\gamma\omega}\eta_{\theta\beta}h_i^{\ \beta},$$

and

$$\left.\frac{\partial h'^{\alpha}_i}{\partial u^\gamma}\right|_{u=e} = 0 .$$

Expansion of (1.2) while noting the transformation laws of the gauge curvatures under a coordinate transformation yields

$$\begin{aligned} &J\epsilon^{ijkh}\bar{L}_{\alpha\beta\gamma\omega}F_i^{\ \alpha\beta}{}_j F_k^{\ \gamma\omega}{}_h + J\epsilon^{ijkh}\bar{L}_{\alpha\beta\gamma}F_i^{\ \alpha\beta}{}_j F_k^{\ \gamma}{}_h \\ &\quad + J\epsilon^{ijkh}\bar{L}_{\alpha\beta}F_i^{\ \alpha}{}_j F_k^{\ \beta}{}_h + \bar{L}^{ij}_{\alpha\beta}J_i^a J_j^b F_a^{\ \alpha\beta}{}_b \\ &\quad + \bar{L}^{ij}_\alpha J_i^a J_j^b F_a^{\ \alpha}{}_b + \bar{L}_0 \qquad (3.5) \\ &= J(\epsilon^{ijkh}L_{\alpha\beta\gamma\omega}F_i^{\ \alpha\beta}{}_j F_k^{\ \gamma\omega}{}_h + \epsilon^{ijkh}L_{\alpha\beta\gamma}F_i^{\ \alpha\beta}{}_j F_k^{\ \gamma}{}_h \\ &\quad + \epsilon^{ijkh}L_{\alpha\beta}F_i^{\ \alpha}{}_j F_k^{\ \beta}{}_h + L^{ij}_{\alpha\beta}F_i^{\ \alpha\beta}{}_j + L^{ij}_\alpha F_i^{\ \alpha}{}_j + L_0) . \end{aligned}$$

In order to determine the gauge transformation laws of the undetermined quantities we expand (1.3), while making use of (2.1) and (2.2), and obtain

$$\begin{aligned} &\epsilon^{ijkh}L'_{\alpha\beta\gamma\omega}\mathcal{L}^\alpha_\mu\mathcal{L}^\beta_\nu\mathcal{L}^\gamma_\sigma\mathcal{L}^\omega_\tau F_i^{\ \mu\nu}{}_j F_k^{\ \sigma\tau}{}_h \\ &\quad + \epsilon^{ijkh}L'_{\alpha\beta\gamma}\mathcal{L}^\alpha_\mu\mathcal{L}^\beta_\nu\mathcal{L}^\gamma_\sigma\eta_{\tau\omega}l^\omega_\phi u^\phi F_i^{\ \mu\nu}{}_j F_k^{\ \sigma\tau}{}_h \\ &\quad + \epsilon^{ijkh}L'_{\alpha\beta\gamma}\mathcal{L}^\alpha_\mu\mathcal{L}^\beta_\nu\mathcal{L}^\gamma_\sigma F_i^{\ \mu\nu}{}_j F_k^{\ \sigma}{}_h \\ &\quad + \epsilon^{ijkh}L'_{\alpha\beta}\mathcal{L}^\alpha_\mu\eta_{\nu\omega}l^\omega_\phi u^\phi\mathcal{L}^\beta_\sigma\eta_{\tau\gamma}l^\gamma_\theta u^\theta F_i^{\ \mu\nu}{}_j F_k^{\ \sigma\tau}{}_h \\ &\quad + 2\epsilon^{ijkh}L'_{\alpha\beta}\mathcal{L}^\alpha_\mu\eta_{\nu\omega}l^\omega_\phi u^\phi\mathcal{L}^\beta_\sigma F_i^{\ \mu\nu}{}_j F_k^{\ \sigma}{}_h \qquad (3.6) \\ &\quad + \epsilon^{ijkh}L'_{\alpha\beta}\mathcal{L}^\alpha_\mu\mathcal{L}^\beta_\nu F_i^{\ \mu}{}_j F_k^{\ \nu}{}_h + L'^{ij}_{\alpha\beta}\mathcal{L}^\alpha_\mu\mathcal{L}^\beta_\nu F_i^{\ \mu\nu}{}_j \\ &\quad + L'^{ij}_\alpha\mathcal{L}^\alpha_\mu\eta_{\nu\beta}l^\beta_\phi u^\phi F_i^{\ \mu\nu}{}_j + L'^{ij}_\alpha\mathcal{L}^\alpha_\mu F_i^{\ \mu}{}_j + L'_0 \\ &= \epsilon^{ijkh}L_{\alpha\beta\gamma\omega}F_i^{\ \alpha\beta}{}_j F_k^{\ \gamma\omega}{}_h + \epsilon^{ijkh}L_{\alpha\beta\gamma}F_i^{\ \alpha\beta}{}_j F_k^{\ \gamma}{}_h \\ &\quad + \epsilon^{ijkh}L_{\alpha\beta}F_i^{\ \alpha}{}_j F_k^{\ \beta}{}_h + L^{ij}_{\alpha\beta}F_i^{\ \alpha\beta}{}_j + L^{ij}_\alpha F_i^{\ \alpha}{}_j + L_0 . \end{aligned}$$

We begin by observing from (3.5) and (3.6) that

$$\bar{L}_0 = JL_0 \quad \text{and} \quad L'_0 = L_0 .$$

Consider instead the quantity

$$B_0 \equiv L_0/h ,$$

which then has the transformation laws

$$\bar{B}_0 = B_0 , \qquad (3.7)$$

and

$$B'_0 = B_0 . \qquad (3.8)$$

Differentiation of (3.7) with respect to J^a_b, followed by evaluation at the identity transformation, $J^r_s = \delta^r_s$, yields

$$(\partial B_0/\partial h_b^{\ a})h_a^{\ \alpha} = 0 .$$

When the above is multiplied by $h_\gamma^{\ a}$ it is found that

$$\partial B_0/\partial h_b^{\ \alpha} = 0 .$$

We have actually established the following lemma.

Lemma 3.1: If a quantity

$$B = B(h_i^{\ \alpha})$$

is a scalar under a coordinate transformation, i.e.,

$$\bar{B} = B,$$

then

$$\partial B/\partial h_i^{\ \alpha} \equiv 0 .$$

In view of (3.8) we then have the following corollary.

Corollary 3.1: If a quantity

$$B_0 = B_0(h_i^{\ \alpha})$$

is a scalar under both coordinate and Poincaré gauge transformations, i.e.,

$$\bar{B}_0 = B_0 \quad \text{and} \quad B'_0 = B_0 ,$$

then

$$B_0 = c ,$$

where c is an arbitrary constant.

Thus we must have that

$$L_0 = ch ,$$

where c is an arbitrary constant.

Next we shall determine $L_{\alpha\beta}$, which, according to (3.5) and (3.6), transforms as

$$\bar{L}_{\alpha\beta} = L_{\alpha\beta} , \qquad (3.9)$$

and

$$L'_{\rho\nu}\mathcal{L}^\rho_\mu\mathcal{L}^\nu_\beta = L_{\mu\beta} . \qquad (3.10)$$

By virtue of (3.9) and Lemma 3.1 we see that

$$\partial L_{\alpha\beta}/\partial h_i^{\gamma} \equiv 0 .$$

When (3.10) is differentiated with respect to $u^{\alpha\phi}$ and then evaluated at $u = e$, we obtain

$$-\tfrac{1}{2}L_{\rho\beta}\delta^{\rho\theta}_{\alpha\phi}\eta_{\theta\mu} - \tfrac{1}{2}L_{\mu\nu}\delta^{\nu\theta}_{\alpha\phi}\eta_{\theta\beta} = 0 .$$

Therefore,

$$L_{\alpha\beta}\eta_{\phi\mu} - L_{\phi\beta}\eta_{\alpha\mu} + L_{\mu\alpha}\eta_{\phi\beta} - L_{\mu\phi}\eta_{\alpha\beta} = 0 .$$

When this is multiplied by $\eta^{\phi\mu}$ it is found that

$$3L_{\alpha\beta} + L_{\beta\alpha} = (\eta^{\phi\mu}L_{\mu\phi})\eta_{\alpha\beta} .$$

However, the quantity $\eta^{\phi\mu}L_{\mu\phi}$ satisfies the hypothesis of Corollary 3.1 and thus

$$3L_{\alpha\beta} + L_{\beta\alpha} = b\eta_{\alpha\beta} ,$$

where b is an arbitrary constant. Antisymmetrization of the above leads to

$$L_{[\alpha\beta]} = 0 , \tag{3.11}$$

and hence

$$L_{\alpha\beta} = d\eta_{\alpha\beta} , \tag{3.12}$$

where d is an arbitrary constant. Note that (3.11) was obtained merely as a consequence of the transformation laws even though the structure of L also demanded it. We have thus established the following lemma.

Lemma 3.2: If a quantity

$$B_{\alpha\beta} = B_{\alpha\beta}(h_i^{\gamma}) ,$$

has the transformation laws

$$\bar{B}_{\alpha\beta} = B_{\alpha\beta}$$

and

$$B'_{\rho\nu}\mathcal{L}^{\rho}_{\mu}\mathcal{L}^{\nu}_{\beta} = B_{\mu\beta} ,$$

then

$$B_{\alpha\beta} = b\eta_{\alpha\beta} ,$$

where b is an arbitrary constant.

In order to calculate $L_{\alpha\beta\gamma}$ we must first establish the following lemma.

Lemma 3.3: If a quantity

$$B_{\alpha} = B_{\alpha}(h_i^{\gamma})$$

has the transformation laws

$$\bar{B}_{\alpha} = B_{\alpha} , \tag{3.13}$$

and

$$B'_{\rho}\mathcal{L}^{\rho}_{\mu} = B_{\mu} , \tag{3.14}$$

then

$$B_{\alpha} \equiv 0 .$$

Proof: Since (3.13) holds, Lemma 3.1 implies that

$$\partial B_{\alpha}/\partial h_i^{\gamma} \equiv 0 .$$

Differentiation of (3.14) with respect to $u^{\alpha\phi}$ followed by evaluation at $u = e$ yields

$$-\tfrac{1}{2}B_{\rho}\delta^{\rho\theta}_{\gamma\phi}\eta_{\theta\mu} = 0 ,$$

and thus,

$$B_{\alpha}\eta_{\phi\mu} - B_{\phi}\eta_{\alpha\mu} = 0 . \tag{3.15}$$

When (3.15) is multiplied by $\eta^{\phi\mu}$ we obtain

$$3B_{\alpha} = 0 ,$$

which establishes the lemma.

From (3.5), (3.6), and (3.12) we see that $L_{\alpha\beta\gamma}$ transforms as

$$\bar{L}_{\alpha\beta\gamma} = L_{\alpha\beta\gamma} \tag{3.16}$$

and

$$L'_{\rho\nu\sigma}\mathcal{L}^{\rho}_{\mu}\mathcal{L}^{\nu}_{\beta}\mathcal{L}^{\sigma}_{\gamma} + 2d\eta_{\tau\sigma}\mathcal{L}^{\tau}_{[\mu}\eta_{\beta]\omega}l^{\omega}_{\phi}u^{\phi}\mathcal{L}^{\sigma}_{\gamma} = L_{\mu\beta\gamma} . \tag{3.17}$$

In view of (3.16) and Lemma 3.1 we have that

$$\partial L_{\alpha\beta\gamma}/\partial h_i^{\mu} \equiv 0 .$$

Differentiation of (3.17) with respect to u^{α} and evaluation at $u = e$ leads to

$$d(\eta_{\mu\gamma}\eta_{\beta\alpha} - \eta_{\beta\gamma}\eta_{\mu\alpha}) = 0 .$$

When this is multiplied by $\eta^{\mu\gamma}$ we obtain

$$3d\eta_{\beta\alpha} = 0 ,$$

and hence

$$d = 0 ,$$

which implies that

$$L_{\alpha\beta} \equiv 0 .$$

Now (3.17) reduces to

$$L'_{\rho\nu\sigma}\mathcal{L}^{\rho}_{\mu}\mathcal{L}^{\nu}_{\beta}\mathcal{L}^{\sigma}_{\gamma} = L_{\mu\beta\gamma} . \tag{3.18}$$

When (3.18) is differentiated with respect to $u^{\alpha\phi}$ and then evaluated at $u = e$, it is found that

$$-\tfrac{1}{2}L_{\rho\beta\gamma}\delta^{\rho\theta}_{\alpha\phi}\eta_{\theta\mu} - \tfrac{1}{2}L_{\mu\nu\gamma}\delta^{\nu\theta}_{\alpha\phi}\eta_{\theta\beta} - \tfrac{1}{2}L_{\mu\beta\sigma}\delta^{\sigma\theta}_{\alpha\phi}\eta_{\theta\gamma} = 0 .$$

Therefore,

$$L_{\alpha\beta\gamma}\eta_{\phi\mu} - L_{\phi\beta\gamma}\eta_{\alpha\mu} + L_{\mu\alpha\gamma}\eta_{\phi\beta} - L_{\mu\phi\gamma}\eta_{\alpha\beta} + L_{\mu\beta\alpha}\eta_{\phi\gamma} - L_{\mu\beta\phi}\eta_{\alpha\gamma} = 0 , \tag{3.19}$$

which, when multiplied by $\eta^{\phi\mu}$, yields

$$3L_{\alpha\beta\gamma} + L_{\beta\alpha\gamma} + L_{\gamma\beta\alpha} = (\eta^{\phi\mu}L_{\mu\phi\gamma})\eta_{\alpha\beta} + (\eta^{\phi\mu}L_{\mu\beta\phi})\eta_{\alpha\gamma} .$$

However, Lemma 3.3 implies that both $\eta^{\phi\mu}L_{\mu\phi\gamma}$ and $\eta^{\phi\mu}L_{\mu\beta\phi}$ vanish and thus

$$3L_{\alpha\beta\gamma} + L_{\beta\alpha\gamma} + L_{\gamma\beta\alpha} = 0 . \tag{3.20}$$

We are now forced to actually use a symmetry property of $L_{\alpha\beta\gamma}$, viz.,

$$L_{\beta\alpha\gamma} = -L_{\alpha\beta\gamma} .$$

This reduces (3.20) to

$$L_{\alpha\beta\gamma} = -\tfrac{1}{2}L_{\gamma\beta\alpha} ,$$

which, when applied twice, yields

$$L_{\alpha\beta\gamma} = \tfrac{1}{4}L_{\alpha\beta\gamma} ,$$

and therefore

$$L_{\alpha\beta\gamma} = 0 .$$

We have thus established the following lemma.

Lemma 3.4: If a quantity

$$B_{\alpha\beta\gamma} = B_{\alpha\beta\gamma}(h_i^{\ \mu})$$

has the antisymmetry

$$B_{\beta\alpha\gamma} = -B_{\alpha\beta\gamma}$$

and the transformation laws

$$\bar{B}_{\alpha\beta\gamma} = B_{\alpha\beta\gamma}$$

and

$$B'_{\rho\nu\sigma}\mathcal{L}^{\rho}_{\ \mu}\mathcal{L}^{\nu}_{\ \beta}\mathcal{L}^{\sigma}_{\ \gamma} = B_{\mu\beta\gamma}\,,$$

then

$$B_{\alpha\beta\gamma} \equiv 0\,.$$

For the quantity $L_{\alpha\beta\gamma\omega}$ the transformation laws obtained from (3.5) and (3.6) are

$$\bar{L}_{\alpha\beta\gamma\omega} = L_{\alpha\beta\gamma\omega}\,, \tag{3.21}$$

and

$$L'_{\rho\nu\sigma\tau}\mathcal{L}^{\rho}_{\ \mu}\mathcal{L}^{\nu}_{\ \beta}\mathcal{L}^{\sigma}_{\ \gamma}\mathcal{L}^{\tau}_{\ \omega} = L_{\mu\beta\gamma\omega}\,. \tag{3.22}$$

From (3.21) and Lemma 3.1 we see that

$$\partial L_{\alpha\beta\gamma\omega}/\partial h_i^{\ \mu} \equiv 0\,.$$

When (3.22) is differentiated with respect to $u^{\alpha\phi}$ and then evaluated at $u = e$, we obtain

$$-\tfrac{1}{2}L_{\rho\beta\gamma\omega}\delta^{\rho\theta}_{\alpha\phi}\eta_{\theta\mu} - \tfrac{1}{2}L_{\mu\nu\gamma\omega}\delta^{\nu\theta}_{\alpha\phi}\eta_{\theta\beta} - \tfrac{1}{2}L_{\mu\beta\sigma\omega}\delta^{\sigma\theta}_{\alpha\phi}\eta_{\theta\gamma} - \tfrac{1}{2}L_{\mu\beta\gamma\tau}\delta^{\tau\theta}_{\alpha\phi}\eta_{\theta\omega} = 0\,.$$

Therefore,

$$L_{\alpha\beta\gamma\omega}\eta_{\phi\mu} - L_{\phi\beta\gamma\omega}\eta_{\alpha\mu} + L_{\mu\alpha\gamma\omega}\eta_{\phi\beta} - L_{\mu\phi\gamma\omega}\eta_{\alpha\beta} + L_{\mu\beta\alpha\omega}\eta_{\phi\gamma} - L_{\mu\beta\phi\omega}\eta_{\alpha\gamma} + L_{\mu\beta\gamma\alpha}\eta_{\phi\omega} - L_{\mu\beta\gamma\phi}\eta_{\alpha\omega} = 0\,, \tag{3.23}$$

which, when multiplied by $\eta^{\phi\mu}$, yields

$$3L_{\alpha\beta\gamma\omega} + L_{\beta\alpha\gamma\omega} + L_{\gamma\beta\alpha\omega} + L_{\omega\beta\gamma\alpha} = (\eta^{\phi\mu}L_{\mu\phi\gamma\omega})\eta_{\alpha\beta} + (\eta^{\phi\mu}L_{\mu\beta\phi\omega})\eta_{\alpha\gamma} + (\eta^{\phi\mu}L_{\mu\beta\gamma\phi})\eta_{\alpha\omega}\,. \tag{3.24}$$

By making use of the antisymmetry properties

$$L_{\alpha\beta\gamma\omega} = -L_{\beta\alpha\gamma\omega} = -L_{\alpha\beta\omega\gamma}\,, \tag{3.25}$$

and Lemma 3.2 it is found that

$$\eta^{\phi\mu}L_{\mu\phi\gamma\omega} = 0\,,$$

$$\eta^{\phi\mu}L_{\mu\beta\phi\omega} = a\eta_{\beta\omega}\,, \tag{3.26}$$

and

$$\eta^{\phi\mu}L_{\mu\beta\gamma\phi} = -a\eta_{\beta\gamma}\,, \tag{3.27}$$

where a is an arbitrary constant. Thus (3.24) reduces to

$$3L_{\alpha\beta\gamma\omega} + L_{\beta\alpha\gamma\omega} + L_{\gamma\beta\alpha\omega} + L_{\omega\beta\gamma\alpha} = a(\eta_{\beta\omega}\eta_{\alpha\gamma} - \eta_{\beta\gamma}\eta_{\alpha\omega})\,. \tag{3.28}$$

When we multiply (3.23) by $\eta^{\phi\gamma}$, while noting (3.25)–(3.27), we obtain

$$L_{\alpha\beta\mu\omega} + L_{\mu\alpha\beta\omega} + 3L_{\mu\beta\alpha\omega} + L_{\mu\beta\omega\alpha} = a(\eta_{\beta\omega}\eta_{\alpha\mu} - \eta_{\mu\omega}\eta_{\alpha\beta})\,. \tag{3.29}$$

Replacing α with γ and μ with α in (3.29) results in

$$3L_{\alpha\beta\gamma\omega} + L_{\alpha\beta\omega\gamma} + L_{\gamma\beta\alpha\omega} + L_{\alpha\gamma\beta\omega} = a(\eta_{\beta\omega}\eta_{\gamma\alpha} - \eta_{\alpha\omega}\eta_{\gamma\beta})\,,$$

which we then subtract from (3.28). With the use of (3.25) we are then able to conclude that

$$L_{\omega\beta\gamma\alpha} = L_{\gamma\alpha\omega\beta}\,. \tag{3.30}$$

By virtue of both (3.25) and (3.30) total antisymmetrization of $L_{\alpha\beta\gamma\omega}$ can be expressed as

$$3L_{[\alpha\beta\gamma\omega]} = -L_{\beta\alpha\gamma\omega} - L_{\gamma\beta\alpha\omega} - L_{\omega\beta\gamma\alpha}\,.$$

Furthermore, since lower case Greek indices range from 1 to 4, $L_{[\alpha\beta\gamma\omega]}$ must be proportional to a Levi–Civita symbol, i.e.,

$$L_{[\alpha\beta\gamma\omega]} = B\epsilon_{\alpha\beta\gamma\omega}\,,$$

where B is a scalar under both coordinate and Poincaré gauge transformations in view of the transformation laws of $\epsilon_{\alpha\beta\gamma\omega}$. Corollary 3.1 restricts B to being a constant. Thus

$$L_{\beta\alpha\gamma\omega} + L_{\gamma\beta\alpha\omega} + L_{\omega\beta\gamma\alpha} = b\epsilon_{\alpha\beta\gamma\omega}\,,$$

where b is an arbitrary constant. Therefore, upon relabeling constants, (3.28) now becomes

$$L_{\alpha\beta\gamma\omega} = a_1\epsilon_{\alpha\beta\gamma\omega} + \tfrac{1}{2}a_2(\eta_{\beta\omega}\eta_{\alpha\gamma} - \eta_{\beta\gamma}\eta_{\alpha\omega})\,,$$

where a_1 and a_2 are arbitrary constants. We have thus established the following lemma.

Lemma 3.5: If a quantity

$$B_{\alpha\beta\gamma\omega} = B_{\alpha\beta\gamma\omega}(h_i^{\ \mu})$$

has the antisymmetries

$$B_{\alpha\beta\gamma\omega} = -B_{\beta\alpha\gamma\omega} = -B_{\alpha\beta\omega\gamma}$$

and the transformation laws

$$\bar{B}_{\alpha\beta\gamma\omega} = B_{\alpha\beta\gamma\omega}$$

and

$$B'_{\rho\nu\sigma\tau}\mathcal{L}^{\rho}_{\ \mu}\mathcal{L}^{\nu}_{\ \beta}\mathcal{L}^{\sigma}_{\ \gamma}\mathcal{L}^{\tau}_{\ \omega} = B_{\mu\beta\gamma\omega}\,,$$

then

$$B_{\alpha\beta\gamma\omega} = a\epsilon_{\alpha\beta\gamma\omega} + b(\eta_{\alpha\gamma}\eta_{\beta\omega} - \eta_{\alpha\omega}\eta_{\beta\gamma})\,,$$

where a and b are arbitrary constants.

It is a relatively simple matter to determine the remaining quantities. The transformation laws for $L_{\alpha}^{\ ij}$ arising from (3.5) and (3.6) are

$$\bar{L}_{\alpha}^{\ ij}J_i^{\ a}J_j^{\ b} = JL_{\alpha}^{\ ab}$$

and

$$L'_{\rho}^{\ ij}\mathcal{L}^{\rho}_{\ \mu} = L_{\mu}^{\ ij}\,.$$

If we consider, instead, the quantity

$$D_{\alpha\beta\gamma} \equiv \frac{1}{h}L_{\gamma}^{\ ij}h_i^{\ \mu}h_j^{\ \nu}\eta_{\mu\alpha}\eta_{\nu\beta}\,,$$

we can apply Lemma 3.4 to $D_{\alpha\beta\gamma}$ since $D_{\alpha\beta\gamma}$ satisfies

$$D_{\beta\alpha\gamma} = -D_{\alpha\beta\gamma}$$

and has the transformation laws

$$\bar{D}_{\alpha\beta\gamma} = D_{\alpha\beta\gamma}$$

and

$$D'_{\rho\nu\sigma}\mathcal{L}^{\rho}_{\mu}\mathcal{L}^{\nu}_{\beta}\mathcal{L}^{\sigma}_{\gamma}=D_{\mu\beta\gamma}\,.$$

Hence

$$D_{\alpha\beta\gamma}\equiv 0\,,$$

and thus

$$L^{ij}_{\alpha}\equiv 0\,.$$

From (3.5) and (3.6) we obtain the transformation laws for $L^{ij}_{\alpha\beta}$, viz.,

$$\bar{L}^{ij}_{\alpha\beta}J^{a}_{i}J^{b}_{j}=JL^{ab}_{\alpha\beta}$$

and

$$L'^{ij}_{\rho\nu}\mathcal{L}^{\rho}_{\mu}\mathcal{L}^{\nu}_{\beta}=L^{ij}_{\mu\beta}\,.$$

Lemma 3.5 can then be applied to the quantity

$$D_{\alpha\beta\gamma\omega}\equiv\frac{1}{h}L^{ij}_{\alpha\beta}h^{\mu}_{i}h^{\nu}_{j}\eta_{\mu\gamma}\eta_{\nu\omega}\,,$$

since it satisfies the required antisymmetries and transformation laws. Therefore $L^{ij}_{\alpha\beta}$ can be expressed as

$$L^{ij}_{\alpha\beta}=hh^{i}_{\mu}h^{j}_{\nu}\eta^{\mu\gamma}\eta^{\nu\omega}[b_1\epsilon_{\alpha\beta\gamma\omega}+\tfrac{1}{2}b_2(\eta_{\alpha\gamma}\eta_{\beta\omega}-\eta_{\alpha\omega}\eta_{\beta\gamma})]\,,$$

where b_1 and b_2 are arbitrary constants. This reduces to

$$L^{ij}_{\alpha\beta}=b_1hh^{i}_{\mu}h^{j}_{\nu}\eta^{\mu\gamma}\eta^{\nu\omega}\epsilon_{\alpha\beta\gamma\omega}+\tfrac{1}{2}b_2h(h^{i}_{\alpha}h^{j}_{\beta}-h^{i}_{\beta}h^{j}_{\alpha})\,.$$

We have thus established the following theorem.

Theorem 3.2: If a Lagrangian of the form

$$L=L(h^{\alpha}_{i};A^{\alpha\beta}_{i},A^{\alpha}_{i};A^{\alpha\beta}_{i,j};A^{\alpha}_{i,j})$$

which has the transformation laws

$$\bar{L}=JL$$

and

$$L'=L$$

is degenerate in the sense that

$$E^{k}_{\sigma\tau}=E^{k}_{\sigma\tau}(h^{\alpha}_{i};h^{\alpha}_{i,j};A^{\alpha\beta}_{i},A^{\alpha}_{i};A^{\alpha\beta}_{i,j};A^{\alpha}_{i,j})$$

and

$$E^{k}_{\sigma}=E^{k}_{\sigma}(h^{\alpha}_{i};h^{\alpha}_{i,j};A^{\alpha\beta}_{i},A^{\alpha}_{i};A^{\alpha\beta}_{i,j};A^{\alpha}_{i,j})\,,$$

then L is restricted to being

$$L=a_1\epsilon^{ijkh}\epsilon_{\alpha\beta\gamma\omega}F_{i}^{\alpha\beta}{}_{j}F_{k}^{\gamma\omega}{}_{h}+a_2\epsilon^{ijkh}\eta_{\alpha\gamma}\eta_{\beta\omega}F_{i}^{\alpha\beta}{}_{j}F_{k}^{\gamma\omega}{}_{h}+b_1hh^{i}_{\mu}h^{j}_{\nu}\eta^{\mu\gamma}\eta^{\nu\omega}\epsilon_{\alpha\beta\gamma\omega}F_{i}^{\alpha\beta}{}_{j}+b_2hh^{i}_{\alpha}h^{j}_{\beta}F_{i}^{\alpha\beta}{}_{j}+ch\,,$$

where a_1, a_2, b_1, b_2, and c are arbitrary constants.

Remark 1: If we look at the full Poincaré group, rather than just the connected component of the identity, then the Levi-Civita symbol $\epsilon_{\alpha\beta\gamma\omega}$ is no longer invariant under a Poincaré gauge transformation, but satisfies

$$\epsilon'_{\alpha\beta\gamma\omega}=\pm\epsilon_{\alpha\beta\gamma\omega}\,.$$

Therefore, if we demand that the Lagrangian be invariant under the full Poincaré group, then L must take the form

$$L=a\epsilon^{ijkh}\eta_{\alpha\gamma}\eta_{\beta\omega}F_{i}^{\alpha\beta}{}_{j}F_{k}^{\gamma\omega}{}_{h}+bhh^{i}_{\alpha}h^{j}_{\beta}F_{i}^{\alpha\beta}{}_{j}+ch\,,$$

where a, b, and c are arbitrary constants.

Remark 2: The Lagrangian depends only on $A^{\alpha\beta}_{i}$ and $A^{\alpha\beta}_{i,j}$. There are no terms involving A^{α}_{i} and $A^{\alpha}_{i,j}$. Thus we are actually dealing with just the Lorentz group. This situation arises from the fact that the transformation law for h^{α}_{i} depends on only $u^{\alpha\beta}$ and not u^{α}.

4. THE FIELD EQUATIONS

We begin our calculations by determining which of the terms in the Lagrangian are divergences since they will have identically vanishing Euler–Lagrange equations. To do so, recall that it is possible to express our Lagrangian in the form

$$L=\epsilon^{ijkh}L_{\Lambda\Sigma}F_{i}^{\Lambda}{}_{j}F_{k}^{\Sigma}{}_{h}+L^{ij}_{\Lambda}(h^{\alpha}_{a})F_{i}^{\Lambda}{}_{j}+L_0(h^{\alpha}_{a})\,.$$

The first term, viz.,

$$L_1\equiv\epsilon^{ijkh}L_{\Lambda\Sigma}F_{i}^{\Lambda}{}_{j}F_{k}^{\Sigma}{}_{h}\,,\tag{4.1}$$

can easily be shown to be a divergence as follows. The Poincaré gauge transformation law for $L_{\Lambda\Sigma}$, viz.,

$$L'_{\Lambda\Sigma}T^{\Lambda}_{\Omega}T^{\Sigma}_{\Gamma}=L_{\Omega\Gamma}\,,$$

where T^{Λ}_{Ω} is the inverse of the adjoint representation, can be differentiated with respect to u^{Ψ} and evaluated at $u=e$ to obtain the invariance identity

$$L_{\Lambda\Gamma}C_{\Omega}{}^{\Lambda}{}_{\Psi}+L_{\Omega\Lambda}C_{\Gamma}{}^{\Lambda}{}_{\Psi}=0\,.\tag{4.2}$$

Expansion of (4.1) in terms of the definition of $F_{i}^{\Lambda}{}_{j}$ leads to

$$L_1=4\epsilon^{ijkh}L_{\Lambda\Sigma}A^{\Lambda}_{i,j}A^{\Sigma}_{k,h}+4\epsilon^{ijkh}L_{\Lambda\Sigma}A^{\Lambda}_{i,j}C_{\Omega}{}^{\Sigma}{}_{\Gamma}A^{\Omega}_{k}A^{\Gamma}_{h}+\epsilon^{ijkh}L_{\Lambda\Sigma}C_{\Psi}{}^{\Lambda}{}_{\Phi}C_{\Omega}{}^{\Sigma}{}_{\Gamma}A^{\Psi}_{i}A^{\Phi}_{j}A^{\Omega}_{k}A^{\Gamma}_{h}\,,$$

which, by using the antisymmetry of ϵ^{ijkh} in each term and (4.2) in the last term, becomes

$$L_1=(4\epsilon^{ijkh}L_{\Lambda\Sigma}A^{\Lambda}_{i}A^{\Sigma}_{k,h})_{,j}+\tfrac{4}{3}\epsilon^{ijkh}L_{\Lambda\Sigma}A^{\Lambda}_{i,j}C_{\Omega}{}^{\Sigma}{}_{\Gamma}A^{\Omega}_{k}A^{\Gamma}_{h}-\tfrac{8}{3}\epsilon^{ijkh}L_{\Lambda\Sigma}A^{\Lambda}_{k,j}C_{\Omega}{}^{\Sigma}{}_{\Gamma}A^{\Omega}_{i}A^{\Gamma}_{h}-\epsilon^{ijkh}L_{\Lambda\Psi}C_{\Sigma}{}^{\Lambda}{}_{[\Phi}C_{\Omega}{}^{\Sigma}{}_{\Gamma]}A^{\Psi}_{i}A^{\Phi}_{j}A^{\Omega}_{k}A^{\Gamma}_{h}\,.\tag{4.3}$$

By relabeling the indices in the second term and using (4.2) in the third term of (4.3), while noting that the last term vanishes by virtue of the Jacobi identity,[3] we find that

$$L_1=(4\epsilon^{ijkh}L_{\Lambda\Sigma}A^{\Lambda}_{i}A^{\Sigma}_{k,h})_{,j}+\tfrac{4}{3}\epsilon^{ijkh}L_{\Omega\Sigma}A^{\Omega}_{i,j}C_{\Lambda}{}^{\Sigma}{}_{\Gamma}A^{\Lambda}_{k}A^{\Gamma}_{h}+\tfrac{8}{3}\epsilon^{ijkh}L_{\Omega\Sigma}A^{\Lambda}_{k,j}C_{\Lambda}{}^{\Sigma}{}_{\Gamma}A^{\Omega}_{i}A^{\Gamma}_{h}$$

which, by virtue of the antisymmetry of ϵ^{ijkh} and $C_{\Lambda}{}^{\Sigma}{}_{\Gamma}$, becomes the divergence

$$L_1=(4\epsilon^{ijkh}L_{\Lambda\Sigma}A^{\Lambda}_{i}A^{\Sigma}_{k,h}+\tfrac{4}{3}\epsilon^{ijkh}L_{\Omega\Sigma}C_{\Lambda}{}^{\Sigma}{}_{\Gamma}A^{\Omega}_{i}A^{\Lambda}_{k}A^{\Gamma}_{h})_{,j}\,.$$

Therefore, we need only calculate the Euler–Lagrange equations for

$$L=b_1hh^{i}_{\mu}h^{j}_{\nu}\eta^{\mu\gamma}\eta^{\nu\omega}\epsilon_{\alpha\beta\gamma\omega}F_{i}^{\alpha\beta}{}_{j}+b_2hh^{i}_{\alpha}h^{j}_{\beta}F_{i}^{\alpha\beta}{}_{j}+ch\,.\tag{4.4}$$

By virtue of the invariance identity corresponding to (4.6) in Ref. 3, viz.,

$$\frac{\partial L}{\partial A^{\sigma\tau}_{k}}+\frac{\partial L}{\partial A^{\alpha\beta}_{l,k}}C_{\gamma\omega}{}^{\alpha\beta}{}_{\sigma\tau}A^{\gamma\omega}_{l}=0\,,\tag{4.5}$$

we can rewrite the Euler–Lagrange expression $E^{k}_{\sigma\tau}$ as

$$E^{k}_{\sigma\tau} = -\frac{\partial L}{\partial A^{\alpha\beta}_{l,k}} C_{\gamma\omega}{}^{\alpha\beta}{}_{\sigma\tau} A_{l}^{\gamma\omega} - \frac{\partial L}{\partial A^{\sigma\tau}_{k,l}}{}_{,l} . \tag{4.6}$$

The invariance identity (4.5) also tells us that any Lagrangian of the form

$$L = L(h_i^{\alpha}; A_i^{\alpha\beta}; A_{i,j}^{\alpha\beta}),$$

must be of the form

$$L = L(h_i^{\alpha}; F_i^{\alpha\beta}{}_j)$$

and

$$\frac{\partial L}{\partial A^{\alpha\beta}_{i,j}} = 2\frac{\partial L}{\partial F_i^{\alpha\beta}{}_j} .$$

Hence (4.6) can be expressed as

$$E^{k}_{\sigma\tau} = -2\frac{\partial L}{\partial F_k^{\sigma\tau}{}_{l}}{}_{\|l} ,$$

where a double vertical bar signifies the double covariant derivative[3,8] using the Christoffel symbol $\{{}_j{}^i{}_k\}$ as the linear connection and $A_i^{\alpha\beta}$ as the Lorentz gauge connection. Thus for the Lagrangian (4.4) we have that

$$E^{k}_{\sigma\tau} = -2b_1 h(h^{k}_{[\mu}h^{l}_{\nu]})_{\|l}\eta^{\mu\gamma}\eta^{\nu\omega}\epsilon_{\sigma\tau\gamma\omega} - 2b_2 h(h^{k}_{[\sigma}h^{l}_{\tau]})_{\|l} .$$

Hence the field equations reduce to

$$b_1 K^{k}_{\mu\nu}\eta^{\mu\gamma}\eta^{\nu\omega}\epsilon_{\sigma\tau\gamma\omega} + b_2 K^{k}_{\sigma\tau} = 0 , \tag{4.7}$$

where

$$K^{k}_{\sigma\tau} \equiv -2h(h^{k}_{[\sigma}h^{l}_{\tau]})_{\|l}$$

is the Euler–Lagrange expression for the Kibble Lagrangian

$$L = hh^{i}_{\alpha}h^{j}_{\beta}F_i^{\alpha\beta}{}_j .$$

When (4.7) is multiplied by $\eta^{\sigma\alpha}\eta^{\tau\beta}\epsilon_{\rho\phi\alpha\beta}$ it is found that

$$-4b_1 K^{k}_{\rho\phi} + b_2 K^{k}_{\sigma\tau}\eta^{\sigma\alpha}\eta^{\tau\beta}\epsilon_{\rho\phi\alpha\beta} = 0 , \tag{4.8}$$

where we have made use of the identities

$$\eta^{\sigma\alpha}\eta^{\tau\beta}\eta^{\mu\gamma}\eta^{\nu\omega}\epsilon_{\sigma\tau\gamma\omega} = -\epsilon^{\alpha\beta\mu\nu} ,$$

and

$$\epsilon^{\alpha\beta\mu\nu}\epsilon_{\rho\phi\alpha\beta} = 2\delta^{\mu\nu}_{\rho\phi} .$$

Notice that (4.7) and (4.8) can be expressed as the matrix equation

$$\begin{bmatrix} b_1 & b_2 \\ b_2 & -4b_1 \end{bmatrix}\begin{bmatrix} K^{k}_{\mu\nu}\eta^{\mu\gamma}\eta^{\nu\omega}\epsilon_{\sigma\tau\gamma\omega} \\ K^{k}_{\sigma\tau} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix},$$

which has only the trivial solution, viz.,

$$K^{k}_{\mu\nu}\eta^{\mu\gamma}\eta^{\nu\omega}\epsilon_{\sigma\tau\gamma\omega} = 0 ,$$

and

$$K^{k}_{\sigma\tau} = 0 ,$$

provided

$$\det\begin{bmatrix} b_1 & b_2 \\ b_2 & -4b_1 \end{bmatrix} \equiv -4b_1{}^2 - b_2{}^2 \neq 0 .$$

Therefore, as long as b_1 and b_2 are not both zero, we recover the Kibble field equations

$$K^{k}_{\sigma\tau} \equiv -2h(h^{k}_{[\sigma}h^{l}_{\tau]})_{\|l} = 0 ,$$

which implies[2] that

$$h^{\alpha}_{i\|j} = 0 .$$

This equation can be used to solve for $A_i^{\alpha\beta}$ in terms of h_i^{α} and $h_{i,j}^{\alpha}$, however, greater use is made of the subsequently vanishing commutator[3]

$$h^{\alpha}_{i\|jk} - h^{\alpha}_{i\|kj} \equiv -R_i{}^{a}{}_{jk}h^{\alpha}_{a} + h^{\gamma}_{i}F_j^{\alpha\beta}{}_k\eta_{\beta\gamma} = 0 ,$$

where $R_i{}^{a}{}_{jk}$ is the Riemann curvature tensor. Thus we can solve for $F_i^{\alpha\beta}{}_j$ as

$$F_i^{\alpha\beta}{}_j = -R_{laij}h^{l}_{\rho}h^{\alpha}_{\sigma}\eta^{\rho\alpha}\eta^{\sigma\beta} . \tag{4.9}$$

The remaining Euler–Lagrange expression for

$$L_2 \equiv hh^{i}_{\mu}h^{j}_{\nu}\eta^{\mu\gamma}\eta^{\nu\omega}\epsilon_{\alpha\beta\gamma\omega}F_i^{\alpha\beta}{}_j ,$$

is

$$\mathscr{E}^{k}_{\phi}(L_2) = hh^{k}_{\phi}h^{i}_{\mu}h^{j}_{\nu}\eta^{\mu\gamma}\eta^{\nu\omega}\epsilon_{\alpha\beta\gamma\omega}F_i^{\alpha\beta}{}_j - 2hh^{i}_{\phi}h^{k}_{\mu}h^{j}_{\nu}\eta^{\mu\gamma}\eta^{\nu\omega}\epsilon_{\alpha\beta\gamma\omega}F_i^{\alpha\beta}{}_j .$$

In view of (4.9) this becomes

$$\mathscr{E}^{k}_{\phi}(L_2) = -hh^{k}_{\phi}h^{i}_{\mu}h^{j}_{\nu}h^{l}_{\rho}h^{a}_{\sigma}\eta^{\mu\gamma}\eta^{\nu\omega}\eta^{\rho\alpha}\eta^{\sigma\beta}\epsilon_{\alpha\beta\gamma\omega}R_{laij} + 2hh^{i}_{\phi}h^{k}_{\mu}h^{j}_{\nu}h^{l}_{\rho}h^{a}_{\sigma}\eta^{\mu\gamma}\eta^{\nu\omega}\eta^{\rho\alpha}\eta^{\sigma\beta}\epsilon_{\alpha\beta\gamma\omega}R_{laij} ,$$

which vanishes by virtue of the identity

$$R_{[la|i|j]} \equiv 0 .$$

For the Lagrangian (4.4) the field equation

$$\mathscr{E}^{k}_{\phi} = 0$$

thus reduces to the Einstein vacuum field equations with cosmological term, i.e.,

$$b_2 R_{ij} = \tfrac{1}{2}cg_{ij} .$$

We have thus established the following theorem.

Theorem 4.1: For a Lagrangian of the form

$$L = L(h_i^{\alpha}; A_i^{\alpha\beta}; A_i^{\alpha}; A_{i,j}^{\alpha\beta}; A_{i,j}^{\alpha})$$

which has the transformation laws

$$\bar{L} = JL$$

and

$$\bar{L} = L$$

and which is degenerate in the sense that

$$E^{k}_{\sigma\tau} = E^{k}_{\sigma\tau}(h_i^{\alpha}; h_{i,j}^{\alpha}; A_i^{\alpha\beta}; A_i^{\alpha}; A_{i,j}^{\alpha\beta}; A_{i,j}^{\alpha})$$

and

$$E^{k}_{\sigma} = E^{k}_{\sigma}(h_i^{\alpha}; h_{i,j}^{\alpha}; A_i^{\alpha\beta}; A_i^{\alpha}; A_{i,j}^{\alpha\beta}; A_{i,j}^{\alpha}) ,$$

the Euler–Lagrange equations, viz.,

$$E^{k}_{\sigma\tau} = 0 , \quad E^{k}_{\sigma} = 0 ,$$

and

$$\mathscr{E}^{k}_{\phi} = 0 ,$$

imply the Einstein vacuum field equations with cosmological term

$$b_2 R_{ij} = \tfrac{1}{2}cg_{ij} ,$$

where b_2 and c are arbitrary constants.

5. DISCUSSION

We have just seen that the properties which we regard

as noteworthy for the Kibble Lagrangian

$$L = hh^{i}{}_{\alpha} h^{j}{}_{\beta} F_{i}{}^{\alpha\beta}{}_{j}$$

are not unique to this Lagrangian. Nonetheless these properties do determine a class of Lagrangians whose field equations give rise to the Einstein vacuum field equations with cosmological term. Since Poincaré gauge invariance arises here only as a consequence of Lorentz gauge invariance, it seems more fitting to call gravity a Lorentz gauge theory. A Poincaré gauge theory should make use of all of the Poincaré group, not just a subgroup.

In view of the success of this approach, an investigation of gauge theories which exhibit invariance under other Lie groups should prove valuable.

ACKNOWLEDGMENTS

I would like to thank Dr. G. W. Horndeski for many fruitful discussions on the material in this paper. I would also like to thank the Natural Sciences and Engineering Research Council of Canada for their financial support.

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Quasi-abelian and fully non-abelian gauge field copies: A classification [a)]

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(Received 8 December 1980, accepted for publication 20 March 1981)

We show that a theorem by S. Solomon on quasi-abelian gauge fields extends to a full classification of ambiguous potentials for any general non-abelian field which exhibits this phenomenon. A characterization for such fields is given, as well as a criterion that distinguishes in a straightforward manner between potentials that are at least locally gauge-equivalent to a fixed canonical potential and those which are not equivalent to that potential anywhere inside a neighborhood of space–time. Our results are obtained for $\mathbb{R}^4$ with an arbitrary non-degenerate metric, but can be easily extended to any space–time. Three examples (due to S. Deser and F. Wilczek, S. Coleman, and T. T. Wu and C. N. Yang) are discussed in order to clarify our analysis.

PACS numbers: 11.10.Np, 11.30.Jw, 02.40.Vh

I. INTRODUCTION

In a recent paper Solomon[1] discussed the geometrical structure of quasi-abelian SU(2) gauge fields. An abelian SU(2) field can be written in the form

$$F_{\mu\nu}(x) = f_{\mu\nu}(x)\tau^3 \tag{1.1}$$

in suitable local coordinate systems in $\mathbb{R}^4$, where τ^3 is one of the SU(2) generators. This field is said to be (globally) quasi-abelian if $\det(f_{\mu\nu}) = 0$ on the whole of $\mathbb{R}^4$.

Solomon showed that such fields are basically extensions to $\mathbb{R}^4$ of gauge fields defined (locally at least) on a two-dimensional submanifold of $\mathbb{R}^4$. Such fields present also potential ambiguities, that is, they can be derived from an infinite family of potentials which are not all gauge equivalent.

We give in the present paper a stronger formulation for Solomon's result: we show that quasi-abelian arbitrary gauge fields have locally a very simple constant canonical expression in $\mathbb{R}^4$, which is obtained as a consequence of the Darboux theorem.[2] All other results in Solomon's paper are obtained out of this canonical form for a quasi-abelian field. Our discussion centers around finite-dimensional semi-simple gauge groups, a class which includes the symmetry groups in practically all current gauge-theoretical models.

Some aspects of quasi-abelian fields can be generalized to include a large class of non-abelian gauge fields, of which an important example is given by Coleman's plane wave solutions for the gauge equations.[3]

In Sec. 2 of this paper we state and prove our generalization of Solomon's theorem: quasi-abelian gauge fields can be locally represented in a suitable coordinate system by a Lie-algebra-valued two-form which has a single constant component. A complete classification is also given for its potentials, which are infinite in number. They are partitioned into two mutually exclusive classes. The first one is generated in a very precise sense by the field's stability group, and consists of all potentials which are gauge equivalent to a fixed canonical potential. The second class consists of all potentials which are not equivalent to any element of the previous class. They are also classified with the help of the algebraic objects involved, and are given a simple characterization. Global smoothness is also an important difference between the two classes. Those of which are equivalent to the canonical potential can be always smoothed out over the manifold; those of which are not can be made smooth only in some specific cases.

Quasi-abelian fields are shown to be particular examples of what is here called a gauge field with a type I degeneracy. In Sec. 3 of this paper we show that the basic features of quasi-Abelian fields are easily generalized to the more general, non-abelian, class of type I fields. We again have two non-intersecting families of potentials which are generated and classified as in the quasi-abelian situation.

The main differences between the two situations are that we lose the simple form for the field when we pass over to the non-abelian case, and that the set of potentials equivalent to the canonical potential may have just one element, the canonical potential itself. Here we reach the most anomalous situation of all: a field which has an infinite system of potentials, none of which can be gauge-transformed over any of the others. An example of this phenomenon is given by Coleman's plane waves.

At the end of Sec. 3 we show that our previous results lead very naturally to a general characterization for fields with potential ambiguities: these are fields which have a type I or type II degeneracy, or, more generally, for which we have the vanishing of $\det {}^*\mathcal{F}$ on a nonvoid open set in $\mathbb{R}^4$. ${}^*\mathcal{F}$ is a familiar matrix in gauge field theory, described below. Since its degeneracy was already known to be a necessary condition for the existence of potential ambiguities in a gauge field, the results of this section show it to be both necessary *and sufficient.*

Finally, in Sec. 4 we discuss three examples of gauge field copies in the light of the previous analysis. These are the Deser and Wilczek infinite family of potentials for a quasi-abelian field,[4] Coleman's plane waves,[3] and the example that started it all, the given one by Wu and Yang.[5]

Our discussion shows that potential ambiguity is a feature of non-abelian gauge fields which can be related to other aspects of such objects[6] but whose specific meaning is still unclear.

[a)] Partially supported by MEC and CNPq (Brazil).

 0022-2488/81/122943-09$01.00

2. SOLOMON'S THEOREM

In what follows we work with objects defined on $\mathbb{R}^4$. Greek indices range from 1 to 4 (or from 0 to 3), while the latin indices i, j, k, are used to designate coordinate systems in a three submanifold of $\mathbb{R}^4$. Also a "0" subscript will be sometimes used to single out a particular coordinate direction in $\mathbb{R}^4$, without any reference to a specific metric signature or physical interpretation, such as the identification of that particular coordinate with "time".

We also suppose that $\mathbb{R}^4$ is endowed with a nondegenerate Minkowskian or Euclidean metric tensor. This has the purpose of simplifying our notation, by allowing some more ease in the manipulation of vectorial indices. It is, however, easily verified that this particular nondegenerate metric has no bearing on our results.

We have as gauge group G a semi-simple finite-dimensional Lie group with Lie algebra $L(G)$, which is spanned by the E^a, which satisfy $[E^a, E^b]_- = c^{abc}E^c$. $a, b, c, d\cdots$ denote Lie algebra components. The group of gauge transformations $\mathcal{G}$ is formed by smooth mappings $u:\mathbb{R}^4\to G$; its relation to the gauge group is discussed in Sec. 3. We will also consider some of its subgroups.

All objects are supposed to be smooth unless otherwise specified, and all $\mathbb{R}^4$-defined numerical functions are supposed to be real. We will in general work in a local coordinate system $\mathbb{R}^4$ and in the trivial bundle $\mathbb{R}^4\times G$. Global results will be always made explicit.

We now give some definitions.

We say that a gauge field $F_{\mu\nu}$ is *abelian* (*locally* on a nonvoid open set $U\subset\mathbb{R}^4$ or *globally* if $U=\mathbb{R}^4$) if it can be written as

$$F_{\mu\nu}(x) = f_{\mu\nu}(x)E \tag{2.1}$$

in a local coordinate system in $U\subset\mathbb{R}^4$, where E is a fixed element of $L(G)$ and the $f_{\mu\nu}$ are components of a nondegenerate two-form on $\mathbb{R}^4$, that is, $\det(f_{\mu\nu}(x))\neq 0$ on a dense subset of $\mathbb{R}$.

We say that a gauge field $F_{\mu\nu}$ is locally (globally) *quasi-abelian* when it has the form (2.1) over a nonvoid open $U\subset\mathbb{R}^4$ (over $\mathbb{R}^4$) and $f_{\mu\nu}$ is degenerate, that is, $\det(f_{\mu\nu})=0$ on U (on $\mathbb{R}^4$).

A general (abelian or non-abelian) gauge field can be written as

$$F_{\mu\nu}(x) = F^a_{\mu\nu}(x)E^a \tag{2.2}$$

in a local coordinate system. A general gauge field is *copied* (or has a potential ambiguity) over U (over $\mathbb{R}^4$) if it can be derived from at least two potentials A^1 and A^2 which differ on U (on $\mathbb{R}^4$). One of these potentials is always supposed to be smooth.

The dual adjoint field matrix ${}^*\mathcal{F}$ is defined (in a local coordinate system):

$${}^*\mathcal{F} = (c^{abc}{}^*f^b_{\mu\nu}(x)). \tag{2.3}$$

where ${}^*f_{\mu\nu} = (1/2)\varepsilon_{\mu\nu\rho\sigma}f^{\rho\sigma}$.

A gauge field F is *degenerate of class I* over an open set $U\subset\mathbb{R}^4$ if there exists a nonvanishing smooth vectorfield $X=(X^\mu)$ on U such that

$${}^*\mathcal{F}(X)=0,$$

or

$${}^*\mathcal{F}^{ab}_{\mu\nu}X^\nu = 0. \tag{2.4}$$

F is *degenerate of class II* over an open $U\subset\mathbb{R}^4$ if there exists a nonvanishing smooth Lie-algebra valued function $\theta:U\to L(G)$, $\theta^a(x)=\theta^a(x)E^a$, such that

$${}^*\mathcal{F}(\theta)=0,$$

$$\mathcal{F}^{ab}_{\mu\nu}\theta^b = 0. \tag{2.5}$$

We notice that if F is degenerate both of class I and II, a solution for ${}^*\mathcal{F}(\xi)=0$ has the form of a linear combination $\Sigma\theta^a X^\mu$ of products of solutions of both classes.

We can now state:

Proposition 2.1: $F_{\mu\nu}$ is a quasi-abelian over an open nonvoid $U\subset\mathbb{R}^4$ iff it is degenerate of class I over U and if it can be written in the form (2.1) over U.

In our version Solomon's theorem has the following form:

Theorem 1: Let F be quasi-abelian over $U\subset\mathbb{R}^4$. Then there exists a nonvoid $V\subseteq U$ and a coordinate system (x^μ) in V such that in V and in this particular system

(i) We can write

$$F_{12}(x) = E \tag{2.6}$$

for a fixed $E\in L(G)$. All other components vanish.

(ii) F has in V, in this special coordinate system, a potential A given by

$$A_1(x) = -(x^2)E \tag{2.7}$$

while $A_2 = A_3 = A_4 = 0$. A is called the *canonical potential* for F.

Let $\mathcal{G}$ be the group of gauge transformations which act on F and A. Let $\mathcal{G}_F$ be the stability group of F, that is,

$$\mathcal{G}_F = \{g\in\mathcal{G}\,|\,g^{-1}F_{\mu\nu}g = F_{\mu\nu}\}.$$

Then

(iii) Potentials for F which are gauge-equivalent to the canonical potential A have the form

$$A(x,g) = A + g^{-1}dg,\ g\in\mathcal{G}_F, \tag{2.8}$$

with $A(x,1)=A$. Moreover, A and A' are gauge-equivalent and are potentials for F iff $A'-A$ comutes with F.

Let $L[C(E)]$ be the set of all objects in $L(G)$ which commute with E; define $B(E)=L(G)/L[C(E)]$ and consider smooth functions $h:\mathbb{R}\to B(E)$, which are then extended to V by writing $H(x)=H(x^1,0,0,0)=h(x^1)$, $x\in V$. We have

(iv-a) Given $H(x)$ as above we have a single family of potentials which are not gauge-equivalent to A,

$$\bar{A}_1(x,H,g) = A_1 + g^{-1}Hg + g^{-1}\partial_1 g,$$

$$\bar{A}_i = g^{-1}\partial_i g,\ g\in\mathcal{G}_F,\ i\neq 1. \tag{2.9}$$

Now consider functions $k:\mathbb{R}^2\to B(E)$ and extend them to V by defining $K(x)=K(x^1,x^2,0,0)=k(x^1,x^2)$. We have:

(iv-b) If $\bar{A}-A=(K_1,K_2,0,0)$, K_1 and $K_2\neq 0$, then there exists a gauge transformation $u(x^1,x^2,0,0)$ such that $u(\bar{A})=\bar{A}'=(\bar{A}'_1,0,0,0)$, and if $\mathcal{G}_F$ is the stability group of F, then the orbit of $\bar{A}$ under the action of $\mathcal{G}_f$ is the collection of all potentials for F which are gauge equivalent to $\bar{A}$.

(v) The objects described in (iii) and (iv) exhaust all potentials for F.

As we will see in Sec. 3, Solomon's theorem lists all the

interesting features of the field copy problem. The classification in (iii) and (iv) is also true in the general case, while there is a straightfoward generalization for (i) and (ii) that mirrors (iv-b).

Solomon's theorem will be proved in a succession of propositions and lemmas.

We will first give a general characterization for (locally or globally) abelian and quasi-abelian fields. Let $E(x)$: $\mathbb{R}^4 \to L(G)$ be a Lie-algebra-valued function and let $f_{\mu\nu}(x)$ be the components of a two-form over $\mathbb{R}^4$ in a given coordinate system. We then assert:

Proposition 2.2: A field gauge F has the form

$$F_{\mu\nu}(x) = f_{\mu\nu}(x)E(x) \tag{2.10}$$

in a local coordinate system iff it is abelian or quasi-abelian in the region where that coordinate system is defined.

The proposition says that if a gauge field can be written as the product of a numerical-valued form by a matrix function, the matrix factor can always be transformed to a constant matrix by a gauge transformation. This result will be generalized below to encompass the case when Eq. (2.10) is a linear combination of fields which does not span the whole Lie algebra.

Proof: Sufficiency. An abelian or quasi-abelian field has the form

$$F_{\mu\nu}(x) = f_{\mu\nu}(x)E \tag{2.11}$$

in a particular coordinate system, and this is clearly a particular case of (2.10).

Necessity. We will show first that there is always a $\mathbb{R}^4$ dependent linear automorphism which sends any object with the form (2.10) over to objects with the form given by (2.11). We then show that such automorphisms can be made to take values in the gauge group G.

We endow $L(G)$ with a nondegenerate inner product and consider the bundle $\mathbb{R}^4 \times L(G)$. For F of the form (2.10), we see that at each point in the coordinate neighborhood, $E(x)$ determines an orthogonal subspace $N(x) \subset L(G)(x)$. One can endow this subspace with a continuous basis which is defined all over the coordinate neighborhood. If this basis is denoted by $X^a(x)$, we can ask that $[X^a, X^b]_-(x) = c^{abc}X^c(x)$, where we have considered $X^1(x) = E(x)$. Rescaling also allows us to put $\|X^a(x)\|^2 = 1$, where the norm is the one induced by the inner product.

We now fix an arbitrary $x_0 \in U$, where U is the coordinate neighborhood where F has the form of Eq. (2.10). Let ξ be the (finite-dimensional) vector space where $L(G)$ is represented and let $GL(\xi)$ be the group of its linear transformations. Then there is a unique $u: U \to GL(\xi)$ (up to a constant factor) such that $X^a(x) = u^{-1}(x)X^a(x_0)u(x)$. If we fix a value for $\det u(x)$, this transformation becomes unique.

We now must show that u can take values inside the gauge group $G \subset GL(\xi)$. Suppose first that G is simple. Let $E \in L(G)$ be an arbitrary object; put $\mathcal{O}_G(E) = \{u^{-1}Eu \mid u \in G\}$, $[\mathcal{O}_G(E)]$, = linear closure $(\mathcal{O}_G(E))$. We can write $L(G) = [\mathcal{O}_G(E)] \oplus N$, where N is a subspace of $L(G)$ unattained by $[\mathcal{O}_G(E)]$. But then the action of G induces on $L(G)$ a direct sum decomposition, which would then imply that G is semi-simple, which is a contradiction. Then $N = 0$, and $[\mathcal{O}_G(E)] = L(G)$. Thus every element of the Lie algebra can be mapped on the direction of every other element.

Now if G is semi-simple, we suppose that F is nonvanishing inside U and that this domain is connected. Thus, due to continuity $E(x)$ will wander inside one of the component subalgebras which add up to form $L(G)$. We then apply the previous reasoning.

The transformations u thus defined are local, since our reasoning has been restricted to a connected $U \subset \mathbb{R}^4$. They can be continuously patched over a connected region where F is abelian (or quasi-abelian). And they can be continuously extended over the whole $\mathbb{R}^4$, since we can continuously extend the basis X^a over the whole manifold.

Proposition 2.2 has been quoted and applied without proof by Solomon[1] in the SU(2) case. It allows one further and immediate generalization, which will be used in Sec. 3. Suppose that F is degenerate of class II on a neighborhood U of $\mathbb{R}^4$. Then over U we have a $L(G)$-valued function $\theta(x)$ such that ${}^*\mathcal{F}(\theta) = 0$. The space of all such θ has a Lie-algebra structure, and so has the complementary commutant space over which $F = f^a(x)E^a$ is defined (to check that $[\theta, \theta']_-$ satisfies the class II degeneracy condition in Eq. (2.5) one uses the Jacobi identity for ${}^*\mathcal{F}([\theta,\theta']_-) = [{}^*f,[\theta,\theta']_-]$).

We denote by $L(H)(x)$ the subalgebra of $L(G)$ over which we define at each point a class II field F. Then

Proposition 2.3: If F is degenerate of class II over $U \subset \mathbb{R}^4$ then there is a subalgebra $L(H) \subset L(G)$ and a gauge transformation u such that $u^{-1}Fu$ takes values only in $L(H)$.

Proof: We first suppose that the space of solutions for ${}^*\mathcal{F}(\theta) = 0, \theta: U \to L(G)$ has constant dimension over U. We then at each point $x \in U$ define a basis for the solutions $\theta(x)$ which satisfies the commutation relations $[X^a, X^b]_-(x) = c^{abc}X^c(x)$, when restricted to the subspace spanned by the $\theta(x)$. We then apply the reasoning of the preceding proposition, while noting that all elements of the basis for the $\theta(x)$ must be in the linear span $[\mathcal{O}_G(E)]$ of a fixed $E \in L(G)$. In order to deal with the case when the space of the $\theta(x)$ does not have a constant dimension over U, we simply choose a basis for $L(G)$ on U which separates at each point the solutions for ${}^*\mathcal{F}\theta = 0$ from objects which are not solutions for it.

This result will be needed in Sec. 3.

Let now $V(x) \subset U(x) \subset \mathbb{R}^4$ be a coordinate neighborhood with coordinates $(x) = (x^\mu) = (x^1, x^2, x^3, x^4)$. In order to avoid trivial situations we suppose that the quasi-abelian field F is non-vanishing on U. In order to prove statement (i) in Theorem 1 we will use the

Lemma 2.4 (*Darboux*): Let f be a closed real two-form on a $(2n + k)$-dimensional manifold M. Let $2n$ be the rank of f. Then for every $x \in M$ there is a coordinate neighborhood and a coordinate system $U(x) \subset M$ such that

$$f|_u = \sum_{i=1}^{n} dx^i \wedge dy^i, \tag{2.12}$$

where $(x) = (x^1, \cdots, x^n, y^1, \cdots y^n, w^1, \cdots, w^k)$.

Proof: See Ref. 2. We can now show that

Proposition 2.5: There is a coordinate neighborhood $V(x) \subset \mathbb{R}^4$ such that the quasi-abelian field F can be written as

as

$$F_{12} = E, \tag{2.13}$$

$$F_{13} = F_{14} = F_{23} = F_{24} = F_{34} = 0. \tag{2.14}$$

This field may be derived from a potential

$$A_1 = -(x^2)E, A_2 = A_3 = A_4 = 0 \tag{2.15}$$

which we call the canonical potential A for F.

Proof: Proposition 2.2 guarantees us that there is a coordinate system inside U where F can be written in the form

$$F_{\mu\nu}(x) = f_{\mu\nu}(x)E, \tag{2.16}$$

$f_{\mu\nu}(x)$ is a real two-form. We apply Darboux's theorem, Proposition 2.4, to it. Since f is a degnerate two-form over a four-dimensional manifold, it must be of rank 2 (since we have excluded the trivial case). Lemma 2.4 and Eq. (2.16) show that we must have

$$F_{12}(x) = E \tag{2.17}$$

as the single surviving component for F, the coordinates being labeled in a convenient manner. The second statement is immediate.

Remark 2.6: We write

$$T = T^3 \oplus 0 = (\epsilon^{3jk} \oplus 0)$$

$$\begin{bmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}. \tag{2.18}$$

(2.13) and (2.14) have the form

$$F = T \otimes E. \tag{2.19}$$

We also notice that $A'_2 = (x^1)E, A'_1 = A'_3 = A'_4 = 0$, is a potential for F in the privileged coordinate system of Proposition 2.5. There is however a local gauge transformation that sends the above potential over the canonical potential A; in the same coordinate system this transformation is given by

$$u(x) = \exp(x^1 x^2)E. \tag{2.20}$$

We finally notice that it is not in general possible to obtain a global coordinate system in $\mathbb{R}^4$ such that F has (globally) the form (2.19), as shown by the following example: let us be given on $\mathbb{R}^2$ the two forms

(A) $f^{(1)} = dx \wedge dy$ in a disk of radius 1 centered at the origin; the coordinate system is rectangular Cartesian.

(B) $f^{(2)} = dr \wedge d\theta$ outside a circle of radius 1/2 centered at the origin, in polar coordinates. $f^{(1)}$ can be derived from a potential $a^{(1)} = x\,dy$, and $f^{(2)}$ from $a^{(2)} = r\,d\theta$, in the respective coordinate systems. Let $g: \mathbb{R}^2 \to \mathbb{R}$ be a smooth function that satisfies $g(r) = 1$ if $r \leqslant 1/2$; $g(r) = 0$ if $r \geqslant 1$ and $\partial g/\partial\theta = 0$. The field f whose potential is

$$a = ga^{(1)} + (1-g)a^{(2)} \tag{2.21}$$

can be written in the annulus $\frac{1}{2} \leqslant r \leqslant 1$ centered at the origin as

$$f = d\,a$$

$$= [rg + (1-g) + r|g_r|(1 - r\cos^2\theta)]dr \wedge d\theta, g_r = \frac{\partial g}{\partial g} \tag{2.22}$$

in polar coordinates. It is easily checked that f is never zero in $\mathbb{R}^2$, and in particular inside the annulus. We notice that f cannot be written in the form (2.19) globally on $\mathbb{R}^2$, since this would imply that there is a transformation that sends Cartesian coordinates over to polar coordinates without singular points. And this is also true when we extend this example in a trivial way to the whole of $\mathbb{R}^4$. This example rose out of a conversation with C. Günther.

We have thus proved (i) and (ii) in Theorem 1. In order to proceed we are going to use two well-known results in the theory of copied fields. We suppose that F is a general non-abelian gauge field over $\mathbb{R}^4$ with potentials A^1 and A^2 which differ on a nonvoid open $U \subset \mathbb{R}^4$.

Proposition 2.7: If F has two potentials which differ on U, then the determinant of the dual adjoint field matrix ${}^*\mathcal{F}$,

$$\det({}^*\mathcal{F}) = 0 \tag{2.23}$$

on U [see Eq. (2.3)].

Also, F has two potentials A^1 and A^2 which differ on U iff A^1 and $A^2 - A^1 = \rho$ satisfies

$$\partial_\mu \rho_\nu - \partial_\nu \rho_\mu + [\rho_\mu, \rho_\nu]_- + [A^1_\mu, \rho_\nu]_- - [A^1_\nu, \rho_\mu] = 0 \tag{2.24}$$

on U.

Proof: If F is derived from two potentials, it must satisfy two different Bianchi identities,

$$\partial_\mu {}^*F^{\mu\nu} + [A^1_\mu, {}^*F^{\mu\nu}]_- = 0,$$

$$\partial_\mu {}^*F^{\mu\nu} + [A^2_\mu, {}^*F^{\mu\nu}] = 0. \tag{2.25}$$

Their difference leads to Eq. (2.23).

Equation (2.24) arises out of the comparison of the fields $F(A^1) = F(A^1 + \rho)$.

The whole problem in the field copy question concerns the classification and existence of solutions for (2.24). The above conditions have been long known.[4,6,7] What we will do next is to classify the solutions for the (algebraic) condition (2.23) and to take them into Eq. (2.24). This will be seen to work also in the general situation, as we show in the next section and in Theorems 2 and 3.

Suppose now that we are inside the privileged coordinate domain and coordinate system where F has the form of Eq. (2.19). ${}^*\mathcal{F}$ can be written here

$${}^*\mathcal{F} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & E^{ad} \\ 0 & 0 & -E^{ad} & 0 \end{bmatrix}, \tag{2.26}$$

where E^{ad} is the adjoint representation of E, that means, the representation of E in the space spanned by the $(c^{ab})^c$. A look at Eq. (2.26) shows that F has both type I and type II degeneracies. The type I solutions are those of the form $\rho = (\rho_1, 0, 0, 0)$ and $\sigma = (0, \sigma_2, 0, 0)$, where $\rho_1 = \rho_1^a E^a$, and $\sigma_2 = \sigma_2^a E^a$. The type II solutions are all the θ_μ such that $[E, \theta_\mu]_- = 0$. The solutions for (2.24) must be found within the space spanned by these type I and type II Lie-algebra-valued objects.

Type II solutions: We will take here $A^1 = A$, the canonical potential. Thus any object that commutes with E will also commute with A, and as a consequence the commutators in Eq. (2.24) will vanish. It is then easily checked as a consequence that the commutators in Eq. (2.24) will vanish. It is then easily checked that θ_μ will be a solution for Eq. (2.24) if

θ_μ is a vacuum potential, that is, $\theta_\mu = u^{-1}\partial_\mu u$, for $u: V \to G$. We also notice that all such solutions are gauge-related, for we have

$$A^2_\mu - A^1_\mu = [\partial_\mu u + [A^1_\mu, u]_-]$$
$$= u^{-1}\partial_\mu u. \tag{2.27}$$

Thus type II solutions always lead to potential ambiguities which are reducible modulo a (local, over V) gauge transformation.

Type I solutions: We consider first $\rho = (\rho_1, 0, 0, 0)$. If we substitute it into Eq. (2.24), taking $A^1 = A$, we get

$$-\partial_2\rho_1(x) = 0,$$
$$-\partial_3\rho_1(x) = 0,$$
$$-\partial_4\rho_1(x) = 0. \tag{2.28}$$

Thus ρ must be independent of x^2, x^3, and x^4. A solution can be obtained if we choose smooth $h^a: \mathbb{R} \to \mathbb{R}$ and take (inside V) $h^a(x) = h^a(x^1, 0, 0, 0)$ and $\rho(x) = [h(x), 0, 0, 0]$. It is not immediately obvious if this solution is gauge-equivalent to A. We will see below that is is so iff $[h, E]_- = 0$.

The second class of type I solutions is given by $\sigma = (0, \sigma_2, 0, 0)$. This is however equivalent to the preceding case, since we can reason as we did while taking $A^1 = A'$ in Remark 2.6.

We notice that, again, the commutators vanish.

We have thus settled that for a quasi-abelian F the differences between any potential A^2 for F and A (or A') span the nullspace of ${}^*\mathscr{F}$. In order to conclude the proof of (iii), (iv) and (v) we will make precise definitions for some concepts frequently used in gauge theory.

The first such concept is that of *gauge*. A *gauge* is a cross section $\Sigma = (x, u(x)) \subset \mathbb{R}^4 \times G$. The *identity gauge* is defined to be $\Sigma_0 = (x, 1) \subset \mathbb{R}^4 \times G$.

The second such concept concerns the relationship between the group of gauge transformations, $\mathscr{G}$, and the gauge group G. A *gauge transformation* is here supposed to be any smooth map $u: \mathbb{R}^4 \to G$. It acts on a gauge Σ as follows:

Proposition 2.8: We have

$$\Sigma = (x, k(x)) \to \Sigma u(x) = [x, k(x)u(x)]. \tag{2.29}$$

For the proof, see Ref. 8.

A local gauge transformation over $U \subset \mathbb{R}^4$ is just any smooth mapping $u: U \to G$. We consider now the stability group $\mathscr{G}_F$ of a general gauge field F. Let us construct F in the privileged gauge described in Prop. 2.3. Let $C(F)$ denote the set of all elements of G which commute with F, that is, which are such that $g^{-1}F_{\mu\nu}g = F_{\mu\nu}$, for all pairs μ, ν. $C(F)$ is called the centralizer of F in G. Now immediately, in this particular representation for F, the stability group $\mathscr{G}_F$ is the group of all $g: U \to C(F)$.

This definition is tied to a particular gauge. Let us show how it extends to a gauge-independent definition. Let a gauge field F be described (if possible) in the privileged form of Prop. 2.3 over U. For all gauge transformations u over U we *define* the *curvature form* φ associated to F to be the form

$$\varphi(x, u) = u^{-1}(F_{\mu\nu}(x)dx^\mu \wedge dx^\nu)u \tag{2.30}$$

over the bundle $U \times G$. The *connection form* over $U \times G$, α, associated to A, is given by

$$\alpha(x, u) = u^{-1}A_\mu(x)dx^\mu u + u^{-1}du. \tag{2.31}$$

The stability group $\mathscr{G}_F$ is easily checked to be nontrivial iff $C(F)$ is not contained in the center of G; also $\mathscr{G}_F$ does not coincide with the stability group of A, $\mathscr{G}_A$, which is precisely $C(F)$.[8] The existence of $\mathscr{G}_F$ allows us to partition all gauges over U under an equivalence relation given by $\Sigma \sim \Sigma'$ if F is unchanged by the map $\Sigma \to \Sigma'$. It is done as follows: let F be given in the form of Proposition 2.3, which we denote by F_0. We attach F_0 to the identity gauge Σ_0 by forming the pair (F_0, Σ_0). $\mathscr{G}$ acts on this pair according to the usual rules, and this action actually generates the entire curvature form φ associated to F on $U \times G$.

We now notice that $\mathscr{G}_F(F_0, \Sigma_0) = (F_0, \Sigma_0\mathscr{G}_F)$. And for any $u \in \mathscr{G}$, the right cosets $\mathscr{G}_F u$ generate disjoint families of gauges, denoted by $\Sigma_0\mathscr{G}_F u$. In each one of these families the stability group of $u^{-1}F_0u$ is clearly $u^{-1}\mathscr{G}_F u$, and the expression of the curvature is kept fixed under the action of a coset element.

Let us now suppose that F_0 is quasi-abelian, and that A is its canonical potential, in the coordinate system of Prop. 2.5. Their orbit under $\mathscr{G}_F$ is clearly given by all triples $(A + g^{-1}dg, F_0, \Sigma g)$, where $g \in \mathscr{G}_F$. And we notice that if A' is a potential for F_0 which is gauge-related to A, A' must be of the form $A + g^{-1}dg$, $g \in \mathscr{G}_F$. We also observe that $A' - A$ commutes both with A and with F_0. We have thus proved:

Proposition 2.9: Potentials for F which are gauge equivalent to the canonical potential A can be expressed in the privileged coordinate system of Prop. 2.5 by

$$A'(x, g) = A + g^{-1}dg, \tag{2.32}$$

where $g \in \mathscr{G}_f$ and $A(x, 1) = A$. Moreover, A and A' are gauge-equivalent and are potentials for F iff A'-A commutes with F.

This deals with (iii) in Theorem I. Also, this deals with all type II copied potentials, that is, all potentials A' such that $A' - A = \theta$ is a type II solution for ${}^*\mathscr{F}(\theta) = 0$. The type I potentials are dealt with by the next proposition. We write $L(C(F))$ for the Lie algebra of $C(F)$, and given the quotient $B(F) = L(G)/L(C(F))$, we take smooth functions $h: \mathbb{R} \to B(F)$ which we then extend to the coordinate domain V by writing $H(x) = H(x^1, 0, 0, 0) = h(x^1)$. This function is obviously *not* smooth, in general situations, over the whole $\mathbb{R}^4$. We then have:

Proposition 2.10: In $V \subset \mathbb{R}^4$, in the coordinate system of Propostion 2.5, given the $B(F)$-valued function H, we have a unique family of potentials $\bar{A}(x, H, g)$ which are not equivalent to A. This family is given by

$$\bar{A}_1(x, H, g) = A_1 + g^{-1}Hg + g^{-1}\partial_1 g, \tag{2.33}$$
$$\bar{A}_i = g^{-1}\partial_i g, \quad g \in \mathscr{G}_F, i \neq 1. \tag{2.34}$$

In this coordinate system, potentials $\bar{A}$ which are not gauge equivalent to the canonical potential A are characterized by the fact that $\bar{A}$-A does not commute with either F or A.

Proof: The second statement is implied by the last statement in the previous proposition. Equations (2.33) and (2.34) are immediately checked to be potentials for F, and uniqueness is implied by the fact that the above expressions give the whole orbit (F fixed) of the potential $\bar{A}(x, H, 1)$.

This deals with assertion (iv-a) in Theorem 1. We must now consider linear combinations of type I and type II solu-

tions. We first suppose that in the privileged coordinate system of Proposition 2.5 we have $\bar{A}\text{-}A = (\rho_1,\rho_2,0,0)$, where $A = (-x^2E,0,0,0)$. If ρ_2 is of type II and ρ_1 is of type I, a gauge transformation that commutes with E is enough to send this potential over to the one in Proposition 2.10.

If $\bar{A}\text{-}A = (\rho_1,\rho_2,0,0)$, ($\rho_1$ and ρ_2 both being of class I) Prop. 2.7 and Eq. (2.24) ensure that ρ_1 and ρ_2 are functions only of x^1 and x^2. Thus there is a (local) gauge transformation $u(x^1,x^2,0,0)$ such that ρ_2 is made to vanish. We are thus left with a potential $u(\bar{A}) = \bar{A}' = (\rho_1',0,0,0)$. Since $F_{12} = E$ is mapped over $F'_{12} = u^{-1}(x^1,x^2)Eu(x^1,x^2)$ in this new gauge (and since all other components remain equal to zero in this new gauge there exists a potential $B(x^1,x^2,0,0) = (B_1,0,0,0)$ given by

$$B_1(x^1,x^2,0,0) = -x^2\int_0^1 u^{-1}(tx^1,tx^2)Eu(tx^1,tx^2)\,dt. \quad (2.35)$$

We notice that $B \neq \bar{A}$ in general; they coincide iff u commutes with E, and this is not the case. If we put $\bar{\rho} = \bar{A}'\text{-}B$, by applying Prop. 2.7 and Eq. (2.24) we check that $\bar{\rho} = \bar{\rho}(x^1,0,0,0)$.

Finally if $\bar{A}\text{-}A = \rho + \theta$, where $\rho = (\rho_1,\rho_2,0,0)$ is of type I, and $\theta = (\theta_1,\theta_2,\theta_3,\theta_4)$ is of type II, we notice that since F has a single component, there is a gauge transformation that sends $\bar{A}$ over $\bar{A} = (A_1',0,0,0)$. (The other components must be the components of a vacuum field.) We then apply the reasoning above and conclude:

Proposition 2.11: Assertion (iv-b) in Theorem 1 is valid.

We also had

Scholium 2.12: In the new gauge of (iv-b) in Theorem 1 the field F' has a potential given by (2.35) which is gauge equivalent to $A' = u(A)$ if and only if u commutes with E.

We thus conclude the proof of Theorem 1.

We now say that F is smoothly copied over $\mathbb{R}^4$ of type I (or II) if it has a smooth potential A' such that the difference $A' - A = \theta$ is a type I (or II solution for ${}^*\mathcal{F}(\theta) = 0$.

Proposition 2.13: F is always smoothly copied of type II.

Proof[6]: Suppose that $\det {}^*\mathcal{F} = 0$ over an open $U \subset \mathbb{R}^4$. Suppose also that F has been written in the gauge given by Proposition 2.2 and consider any smooth function $\theta: \bar{U} \to L(C(F))$. If μ is a real "bump" function for U, that is, a function which is zero on $\mathbb{R}^4 - U$, nonzero on U, and smooth over $\mathbb{R}^4$, we put $g(x) = \exp\mu(x)\theta(x)$, and have the smooth potential $A' = A + g^{-1}dg$ on the whole of $\mathbb{R}^4$.

It is, however, easy to notice that type I solutions are not always smoothly copied on the whole of $\mathbb{R}^4$, since Eqs. (2.33) and (2.34) explicitly depend on the existence of a function which can be extended in a smooth way only in a Cartesian product neighborhood. We can restrict our reasoning to a plane $\mathbb{R}^2$ in $\mathbb{R}^4$, due to (i) in Theorem 1. The function h in Proposition 2.10 is smooth over the line, or any of its subintervals, which we denote by J. It can be globally extended only by the products $J \times \mathbb{R}$ or by $J \times S^1$, and then again by taking the product of this factor with $\mathbb{R}^2$ to get to the dimension of $\mathbb{R}^4$. Thus, if we denote the sets $J \times \mathbb{R}^3$ or $J \times S^1 \times \mathbb{R}^2$ by W, it becomes apparent that a potential $\bar{A}$ is smoothly copied of type II iff the open set U where $\det {}^*\mathcal{F} = 0$ contains a subset diffeomorphic to W such that F has the form of (i) in Theorem 1 in a coordinate system which may be restricted to the whole of W, and where the index 1 denotes the coordinate parallel to J in W.

We can state this result in a less precise version

Proposition 2.14: Type II potentials for quasi-abelian fields are not in general smooth over the whole of $\mathbb{R}^4$.

Thus we conclude our discussion of quasi-Abelian gauge fields and their potentials.

3. CLASS I AND CLASS II NON-ABELIAN GAUGE FIELDS

The proof that we have given for Theorem 1 is a direct consequence of the Darboux theorem in symplectic geometry. However the theorem's statements can be slightly modified so that they can be applied in more general situations. Quasi-abelian fields are abelian fields which have (locally at least) a type I degeneracy. We will now consider a general non-abelian gauge field with a class I degeneracy, that is, such that there is a smooth non-zero vector field X which satisfies

$${}^*\mathcal{F}(X) = 0 \quad (3.1)$$

inside a nonvoid open set U in $\mathbb{R}^4$.

We first suppose that F has no class II degeneracy on $\mathbb{R}^4$. This immediately excludes quasi-abelian fields from the scope of Theorem 2, which we now state.

Theorem 2: Let F be a type I field as characterized above, and let it be degenerate over $U \subset \mathbb{R}^4$. Then

(i) There is a local coordinate domain $V \subset U$ together with an adequate cordinate system such that F can be written as

$$F_{i,0}(x) = \partial_i A_0(x),\ i = 1,2,3,\ x \in V. \quad (3.2)$$

while all other components vanish.

(ii) In that particular coordinate system F can be derived from the potential

$$A(x) = (A_0(x),0,0,0) \quad (3.3)$$

which we call the canonical potential for F in V.

(iii) Let us be given a function $h: \mathbb{R} \to L(G)$; extend it to V by defining $H(x) = H(x^0,0,0,0) = h(x^0)$, in the coordinate syste tem established above. Then the potential $\bar{A}(x) = (A_0(x),0,0,0)$ given by

$$\bar{A}_0(x,H) = A_0 + H \quad (3.4)$$

is a potential for F which is not gauge related to A.

(iv), (ii), and all possible objects as in (iii) exhaust all potentials for F.

Theorem 2 shows that the general class I fields have a potential ambiguity which appears as an extension of the situation described in the quasi-abelian case. Since we have now a fully non-abelian field, all gauge-equivalent potentials collapse over the canonical potential, while the other potentials become unique in the sense that no gauge equivalence is possible among them.

We again split the proof of this theorem into several propositions.

Proposition 3.1: There is a coordinate domain $V \subset U$ and a coordinate system $(x^0,x^i) = (x^0,x^1,x^2,x^3)$ in U such that

$${}^*\mathcal{F}^{ab}_{oi}(x) = 0. \quad (3.5)$$

Proof: On U there is a nonvanishing vector field X such that ${}^*\mathcal{F}(x) = 0$, or in components

$${}^*\mathcal{F}^{ab}_{\mu\nu} X^\nu = 0. \tag{3.6}$$

Let us now write $X = X_0$. Inside U one can then look for three linearly independent vector fields x_i which satisfy

$$[X_i, X_j]_- = [X_i, X_0]_- = 0. \tag{3.7}$$

for all i. In a region where these four X_μ are non-vanishing, they determine a local coordinate system with respect to which their components are $(X_\mu)^\nu = \delta^\nu_\mu$. Since $X_0 = (1,0,0,0)$ is a solution for (3.6), we have in this particular coordinate system

$${}^*\mathcal{F}^{ab}_{\mu\nu}\delta^\nu_0 = 0 \text{ or } {}^*\mathcal{F}^{ab}_{\mu 0} = 0. \tag{3.8}$$

That is, ${}^*\mathcal{F}^{ab}_{i0} = 0$ in this coordinate system over $V \subset U$.

This result implies:

Proposition 3.2: In this particular system in V the field F can be written as

$$F_{i0} = \partial_i A_0, \tag{3.9}$$

$$F_{ij} = 0, \tag{3.10}$$

and has a potential A with components $A(x) = (A_0(x),0,0,0)$.

Proof: Since we have ${}^*\mathcal{F}^{ab}_{i0} = 0$, we have $\mathcal{F}^{ab}_{ij} = 0$. And as $\mathcal{F}^{ac}_{ij} = (c^{abc} f^b_{ij})$, due to the semisimplicity of the group G we conclude that the $F_{ij} = f^b_{ij} E^b = 0$. Thus the only surviving components of the field F in this coordinate system are the F_{oj}. Thus the potential for F, A, splits into $A = (A'_0, A_i)$. The A_i are solely responsible for the components F_{ij} of the field, and these form the components of a vacuum field. Then there is a gauge transformation that sends A_i to zero, and we are left with a single surviving component for A along the x^0 direction, that is, we get $A = (A_0,0,0,0)$, where $A_0(x) = a^b_0(x) E^b$, after performing that gauge transformation.

We have thus proved assertions (i) and (ii) in Theorem 2. Since the field is supposed to be fully non-abelian, no type II degeneracies are allowed, and then the construction indicated in Proposition 2.3 becomes trivial. Thus the stability group of the field is reduced to the identity element, and as a consequence the equivalence class of gauges molulo the stability group $\mathcal{G}_F$ collapses over $(A,F,\Sigma.)$, where A is the canonical potential. As it can be immediately checked that all $\bar{A}(x,H)$ are potentials for F, and that, as a consequence of the previous reasoning, no $\bar{A}$ can be gauge mapped over any other or over A, we conclude the proof of (iii) and (iv) in Theorem II.

We now go back to an observation made at the beginning of Sec. 2, and notice that any solution θ for ${}^*\mathcal{F}(\theta) = 0$, or in components

$${}^*\mathcal{F}^{ab}_{\mu\nu}\theta^{\nu b} = 0 \tag{3.11}$$

must be a linear combination of products of type I and type II solutions, that is $\theta = (\theta^{\nu b}) = (\Sigma' \theta^\nu \theta^b)$, where $\theta^\nu(\theta^b)$ is a type I (type II) solution for (3.11). Theorem 2 shows that all type I solutions lead to copied potentials which are smooth at least over V; Theorem 1 shows that a special class of type I fields are also copied but the potential ambiguity may be reduced modulo a gauge transformation. The reasoning that leads to Proposition 2.9 is, however, general enough to fit in the larger picture. Let F be a general gauge field which has a type I degeneracy over an open $V \subset \mathbb{R}^4$ type II degeneracy over $W \subset \mathbb{R}^4$; we write $U = V \cup W$. Let F be written in the form indicated by Proposition 2.3 whenever possible, that means over W. Let $L(C(F))$ be the commutant subalgebra of $L(H)$ inside $L(G)$, [$L(H)$ is the subalgebra of $L(G)$ where F takes values.] Since dim $L(H)$ may vary over W, we will actually have to cut up this region into the neighborhoods where dim $L(H)$ is constant. It is sufficient, however, to consider just one of these specific domains and then piece things together. We are thus given the stability group $\mathcal{G}_F$ of F and the elements in $L(G)$ which do not commute with some component of F. These are elements of $B(F) = L(G)/L(C(F))$.

We state:

Theorem 3: Let F be degenerate of class I over V, of class II over W; let $U = V \cup W$. In general (cf. Theorem 1) $V \cap W \neq 0$.

(i) There is a local coordinate system on a domain $V' \subset V$ such that F has the form of (i), Theorem 2.

(ii) There is a unique potential of the form (ii), Theorem 2 for the field F. If F is of class II over V', this potential is the unique potential that takes its values inside $L(H)$.

(iii) The potentials for F which are gauge equivalent to the canonical potential A described in (ii) above have the form

$$A'(x,g) = A + g^{-1}dg, \quad g \in \mathcal{G}_F \tag{3.12}$$

and are such that $A' - A$ commutes with F.

(iv) The potentials for F which are not gauge equivalent to A have the form

$$\bar{A}_0(x,H,g) = A_0 + g^{-1}Hg + g^{-1}\partial_0 g, \tag{3.13}$$

$$\bar{A}_i(x,H,g) = g^{-1}\partial_i g, \quad g \in \mathcal{G}_F \tag{3.14}$$

with the notations of (iii), Theorem 2.

(iii) and (iv) are exhaustive.

(v) F has a potential ambiguity on $\mathbb{R}^4$ iff det ${}^*\mathcal{F} = 0$ on a nonvoid open $U \subset \mathbb{R}^4$.

Proof: We suppose that $L(H)$ has a constant dimension over V'. (i) is proved as in Theorem 2, and so it (ii). The argument for (iii) in Theorem 1 applies equally well to the proof of Eq. (3.12), and so does the similar agument for (iv), as well as the exhaustiveness of potentials (iii) and (iv).

(v) is a necessary condition, for Proposition 2.7 (iii) and (iv) show that the differences $A' - A$ and $\bar{A} - A$ span the space of solutions of ${}^*\mathcal{F}(\theta) = 0$. We finally notice the vanishing of det ${}^*\mathcal{F}$ over a set with a void interior in $\mathbb{R}^4$ does not lead to the existence of potential ambiguities, since the nonvanishing of det${}^*\mathcal{F}$ over an open set is a sufficient condition for the existence of a single potential for the field F over that open set, and if det ${}^*\mathcal{F}$ vanishes over a closed set C with a void interior in $\mathbb{R}^4$, $\mathbb{R}^4 - C$ is dense in $\mathbb{R}^4$, and F and its potential can be smoothly and uniquely extended to the whole of $\mathbb{R}^4$.

We notice that the canonical potential for a type II field can be defined as the (unique) lowest-dimensional solution for the linear equation

$$\partial_\mu {}^*f^{a\mu\nu} = {}^*\mathcal{F}^{ab\mu\nu} A^b_\mu. \tag{3.15}$$

which arises out of the differential Bianchi identities for F.

Proposition 3.3: If F is copied of type II over $U \subset \mathbb{R}^4$, then F is smoothly copied over $\mathbb{R}^4$.

Proof: F is smoothly copied if it has at least a smooth potential which does not coincide with the canonical potential. We first partition U into neighborhoods U_i where dim $L(H)$ is constant. We then apply here the reasoning in Proposition 2.11 to each U_i.

Proposition 3.4: F is not always smoothly copied of type I over an arbitrary $U \subset \mathbb{R}^4$.

Proof: The argument runs as in the discussion preceding Proposition 2.12. The geometry for the sets in $\mathbb{R}^4$ which entail a global smoothness for potentials of F which are not equivalent to A is also the same in this case.

4. EXAMPLES

We discuss here three examples from the current literature on the subject in order to clarify our preceding analysis. These are Deser and Wilczek's quasi-abelian field and its infinite family of potentials,[4,9] Coleman's plane waves[3] and the example that started it all, Wu and Yang's.[5]

A. The Deser and Wilczek example

We start our discussions with the slightly more general form that was discussed by Bollini, Giambiagi, and Tiomno.[7,10] Let us be given the trivial bundle $\mathbb{R}^4 \times G$ and the smooth functions

$$\xi : \mathbb{R}^4 \to \mathbb{R},$$
$$A : \mathbb{R} \to L(G),$$
$$f : \mathbb{R} \to \mathbb{R}.$$

In the local coordinate system we choose a constant covector $\eta = (\eta_\mu)$ and define the smooth potentials

$$A(f,x) = \{\eta_\mu + f(\xi)\partial_\mu \xi\} A(\xi). \tag{4.1}$$

In this coordinate system the field is given by

$$F_{\mu\nu}(x) = \{\eta_\nu \partial_\mu \xi - \eta_\mu \partial_\nu \xi\} \partial A / \partial \xi. \tag{4.2}$$

We first apply Proposition 2.2 to (4.2). If we put $\partial A / \partial \xi = -(\partial \lambda / \partial \xi) u(\xi) E u^{-1}(\xi)$, for a fixed $E \in L(G)$ and for a smooth function $\lambda : \mathbb{R} \to \mathbb{R}$, we get in the new gauge

$$F'_{\mu\nu} = u^{-1} F_{\mu\nu} u = (\eta_\nu \partial_\mu \xi - \eta_\mu \partial_\nu \xi)(-\partial \lambda / \partial \xi) E. \tag{4.3}$$

Now since we have

$$\partial_\nu \xi \partial \lambda / \partial \xi = \partial_\nu \lambda \tag{4.4}$$

we can choose (locally at least) the symplectic coordinate system where $\eta = (1,0,0,0)$ and $(\partial_\nu \lambda) = (0,1,0,0)$. Thus (4.3) becomes

$$F_{12} = E, \tag{4.5}$$

while all other components vanish. The family in Eq. (4.1) is given by

$$A_1 = u^{-1}(x^2) A(x^2) u(x^2), \tag{4.6}$$
$$A_2 = f(x^2) u^{-1}(x^2) u(x^2) + u^{-1}(x^2)(\partial_2) u(x^2) \quad (x^2 = \lambda). \tag{4.7}$$

The rest is zero. The reasoning before Proposition 2.11 guarantees us that in the general case these potentials are not mutually gauge equivalent.

B. The Coleman plane waves

Let $\mathbb{R}^4$ be endowed with a Minkowskian metric and out of the standard Cartesian coordinates (x^0, x^i) we define the light cone coordinates $x^\pm = x^0 \pm x^3$, x^1, x^2. Coleman introduced the plane-wave[3] solutions for the gauge field equations

$$A^a_+ = f^+(x^+)x^1 + g^a(x^+)x^2 + h^a(x^+), \tag{4.8}$$
$$A^a_- = A^a_1 = A^a_2 = 0, \tag{4.9}$$

with field strength given by

$$F^a_{1+} = f^a, \tag{4.10}$$
$$F^a_{2+} = g^a. \tag{4.11}$$

These are clearly of the given form in (iii), Theorem 2. We notice that the canonical potential is given by

$$A^0_+ = f(x^+)x^1 + g(x^+)x^2; A^0_- = A^0_1 = A^0_2 = 0 \tag{4.12}$$

and that Eqs. (4.8) and (4.9) are not gauge equivalent to Eq. (4.12), in the general case.

C. The Wu and Yang example[5]

The base manifold here is $\mathbb{R}^3$ minus the nonpositive z axis, times $\mathbb{R}$. The gauge group is supposed to be SO(3), but our reasoning is valid for any finite-dimensional semi-simple group. We will apply Theorem 3 to this case, despite the fact that since the field is quasi-abelian we could have used Theorem 1. Theorem 3 will suffice. The potential is given by

$$A_\phi = [(1 - \cos\theta)/r \sin\theta] E, \tag{4.13}$$
$$A_r = A_\theta = A_t = 0. \tag{4.14}$$

This is the potential for the field of a magnetic monopole sitting at the origin of the coordinate system in $\mathbb{R}^3 \times \mathbb{R}$, where $\mathbb{R}^3$ is described by spherical coordinates. the "bad" region for the potential has been already excluded. This monopole generates a radial magnetic field along the constant gauge direction E, and it is sourceless. It is easy to check that a potential such as

$$\bar{A}_\phi = A_\phi + \phi E', \tag{4.15}$$
$$\bar{A}_r = \bar{A}_\theta = \bar{A}_t = 0, \tag{4.16}$$

will generate the same field as (4.13) and (4.14). It will *not*, however, be sourceless if we ask that $[E,E']_- \neq 0$, and as a consequence of our analysis in Secs. 2 and 3, where nonequivalence is tied to such noncommutativity, the potential above is not equivalent to A.

This was the main point in Wu and Yang's argument.

5. CONCLUSION

We have shown that Solomon's results for quasi-abelian SU(2) fields[1] can be given a stronger and more general formulation for any gauge field where the gauge group is finite-dimensional and semi-simple. The main interest of this extension however lies in that the chief features of quasi-abelian fields are easily generalized to a non-abelian situation. We are thus led to a characterization of gauge fields with potential ambiguity and to a classification of their ambiguity and to a classification of their ambiguous potentials that mirrors the classification obtained in the quasi-abelian case.

The discussion of class II fields on general manifolds

has been done elsewhere;[6] class I fields have then been expressly excluded from our analysis. The present discussion has been restricted to fields on $\mathbb{R}^4$ and over a trivial bundle; it can however be generalized to arbitrary space-times in a straightfoward manner. In particular, it is immediately noticed that space-times that do not admit a subset with the topology of $J \times S^1 \times N$ or $J \times \mathbb{R}$ or $J \times \mathbb{R} \times N$ (cf., Proposition 2.12; N must be a closed boundariless two-submanifold of our general space-time) do not admit a copied potential of type I which can be smoothly extended over the whole space-time.

ACKNOWLEDGMENTS

The author acknowledges an interesting conversation with Christian Günther on symplectic forms over the plane. He also wishes to thank the Department of Mathematics, University of Rochester, and Professor S. L. Segal for their hospitality.

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Democracy of internal symmetries in supersymmetrical quantum field theory

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(Received 11 April 1980; accepted for publication 19 September 1980)

The freedom of choice of some discrete and internal symmetries in the supersymmetric, massive, interacting quantum field theory is discussed. It is shown that the discrete symmetry consisting of changing the sign of some (not all) scalar fields is incompatible with the supersymmetric structure of the theory. It is further demonstrated that an internal symmetry which transforms only some of the fields of fixed spin leaving the other fields invariant and which acts nontrivially on the supercharges can not be admitted as a symmetry; although it can be a good internal symmetry in absence of supersymmetric covariance. Moreover, in case of a model consisting of scalar, spinor, and vector fields even a symmetry which transforms all of the scalar (vector) fields leaving spinor and vector (scalar) fields unaffected is ruled out provided it acts nontrivially on some of the supercharges.

PACS numbers: 11.30.Pb

1. INTRODUCTION

This note is meant as a commentary to an earlier paper written by Haag, Sohnius, and me[1] and is concerned with two problems, which often cause some confusion and misunderstanding.

To begin with, let me remind the reader of two fundamental statements concerning the symmetries and supersymmetries:

(i) The "No Go" theorem of Coleman and Mandula[2] claims that in a quantum theory of a finite number of massive fields which all interact with each other, conforming with the usually accepted axioms, the only admissible S-matrix symmetry generators are those of the Poincaré group and of the group of internal symmetries, the latter commuting with the Poincaré group.

Notice that this theorem does not apply to the case of free fields.

(ii) The *extended* Coleman–Mandula theorem[1] states that in a theory which in addition to the symmetry properties mentioned above displays supersymmetric covariance, the set of admissible generators is enlarged by a finite number of spinorial generators $Q_A^{(L)}$, which we shall call supercharges, (where $A=1,2$ is the spinor index and $L=1, \ldots, N$ labels the supercharges) and their Hermitian conjugates; these supercharges commute with the translations. The Poincaré generators P_μ and $M_{\mu\nu}$, $\mu;\nu=0,1,2,3$, internal symmetry generators B_l, $l=1,\ldots k$, as well as $Q_A^{(L)}$ have to satisfy the following commutation relations[1]:

$$\{Q_A^{(L)}, Q_B^{(M)}\} = c^{LM}(\sigma^\mu)_{A\dot{B}} P_\mu = c^{LM} P_{A\dot{B}} , \tag{1}$$

$$\{Q_A^{(L)}, Q_B^{(M)}\} = \epsilon_{AB} Z^{LM} , \tag{2}$$

$$[Q_A^{(L)}, B_l] = \sum_M s_l^{LM} Q_A^{(M)} , \tag{3}$$

$$[B_l, B_m] = i \sum_k c_{lm}^k B_k ,$$

$$[Q_A^{(L)}, P_\mu] = [B_l, P_\mu] = 0 ,$$

where c^{LM} is a positive definite Hermitian matrix.[3] The operators $P_\mu (\mu=0,1,2,3)$ form the energy-momentum vector of the *whole* system. The central charges $Z^{LM} = -Z^{ML}$ commute with all other generators and so, of course, belong to the center of the algebra of B_l. Under the Lorentz transformation B_l (and Z^{LM}) transform as scalars, P_μ as a vector, and $Q_A^{(L)}$ as spinors. B_l may, but do not have to commute with $Q_A^{(L)}$.

The first rather minor problem, discussed in Sec. 2, is to what extent the definition of the spinorial charge in a field-theoretical setting is unambiguous.

The examination of this question leads us, in a natural way, to the main problem, considered in Secs. 3 and 4, namely: are there any *restrictions* imposed upon the *discrete and internal* symmetries originating from the presence of supersymmetric covariance of a model? The Coleman–Mandula theorem in its original version[2] does not impose any restrictions upon the internal symmetries.[4] The discrete symmetry consisting in changing or preserving the sign of the field, dealt with in Sec. 3, is also not limited by the axioms. As we shall see this is *no longer* the case when we require that the model under consideration exhibits supersymmetric covariance. The restriction comes from relation (1), (2), and (3). Although—given an internal symmetry—one can always find a suitable supersymmetric model of field theory such that these requirements are satisfied, the reverse statement is not true; not every internal or discrete symmetry admissible in a given field theory which does *not* display supersymmetric properties can be implemented in a similar but supersymmetrically covariant theory. The internal or discrete symmetries compatible with the supersymmetric structure of the theory and acting nontrivially on the supercharges must satisfy a kind of *democracy principle* with respect to the fields representing the model; they must act on these fields in a fairly uniform way, without favoring some of them. We shall make this rather vague statement more precise in Secs. 3 and 4.

2. AMBIGUITY OF THE DEFINITION OF SPINORIAL CHARGES

Given a model in field theory, the generators P_μ and $M_{\mu\nu}$ are defined uniquely; there is also no ambiguity in defining the basis of internal charges B_l, although there is considerable freedom in choosing such a basis. Are the supercharges $Q_A^{(L)}$ also defined in a nonambiguous way?

To answer this question let me call to the attention of the reader that the easiest way to investigate the struc-

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ture of the generators is to express them in terms of asymptotic (incoming or outgoing) free fields which we assume for simplicity to be all of the same mass $m \neq 0$ and to form an irreducible set. In terms of these fields the generators are expressed as sesquilinear forms in the creation and annihilation operators. Of course, for the asymptotic free field theory we will find infinitely many generators of numerous free field symmetries among which, however, we shall also, for sure, find the few generators of the S-matrix symmetries chosen by the extended Coleman–Mandula Theorem.

To make things as simple as possible let us start with the case of one supercharge (i.e., $N=1$) and a model consisting of *one* neutral spinor field and *two* real scalar fields.

The free asymptotic—incoming or outgoing—fields belonging to the mass $m \neq 0$ and corresponding to the interacting fields of the model are

$$\psi_A(x)=\left(\frac{1}{2\pi}\right)^{3/2}\int\frac{d^3p}{2\omega_p}\sum_{\sigma=1}^{2}\{\,[p]_A{}^{\sigma}a^+(\sigma)e^{ipx} + i[p]_{A\sigma}a(\sigma)e^{-ipx}\}, \quad A=1,2,$$

$$\varphi^{(i)}(x)=\left(\frac{1}{2\pi}\right)^{3/2}\int\frac{d^3p}{2\omega_p}\{a^{(i)+}e^{ipx}+a^{(i)}e^{-ipx}\}, \quad i=1,2,$$

resp., where $\omega_p=+(\mathbf{p}^2+m^2)^{1/2}$, $[p]_A^{\sigma}$ is the 2×2 boost matrix,[5] $[p]_{A\sigma}=[p]_A{}^{\rho}\epsilon_{\rho\sigma}$, $\epsilon_{\rho\sigma}=\left(\begin{smallmatrix}0&1\\-1&0\end{smallmatrix}\right)$, $px=\omega_p x_0-\mathbf{px}$, and $a(\sigma)\equiv a(\mathbf{p},\sigma)$ and $a^{(i)}\equiv a^{(i)}(\mathbf{p})$ are annihilation operators for the free spinor and scalar fields of mass $m\neq 0$, momentum $\mathbf{p}=(p_1,p_2,p_3)$ and spin $=(\sigma-\frac{1}{2})$ resp.

The free fields satisfy the neutrality (reality) conditions

$$\partial^{A\dot{B}}\psi_A(x)=m\psi^{\dot{B}}(x); \quad \partial^{A\dot{B}}\equiv(\sigma^{\mu})^{A\dot{B}}\partial_{\mu},$$

$$\varphi^{(i)}(x)=\varphi^{(i)*}(x), \quad i=1,2,$$

and the commutation relations

$$\{\psi_A(x),\psi_B(y)\}=-\epsilon_{AB}\Delta(x-y), \quad A,B=1,2,$$

$$[\varphi^{(i)}(x),\varphi^{(j)}(y)]=i\Delta(x-y)\delta^{ij}, \quad i,j=1,2,$$

$$\Delta(x)=-\frac{i}{(2\pi)^3}\int dp\,\delta(p^2-m^2)\epsilon(p_0)e^{-ipx}.$$

All asymptotic fields satisfy the Klein–Gordon equation with mass $m\neq 0$.

In this particular case a straightforward computation shows that among the multitude of translationally invariant spinorial generators which appear in the theory of free asymptotic fields there are—up to the irrelevant phase factor—*two* and *only two* distinct candidates which satisfy (1), viz.,

$$Q_A=\frac{im}{\sqrt{2}}\int\frac{d^3p}{2\omega_p}\sum_{k=1}^{2}c^{(k)}\sum_{\sigma=1}^{2}\{i[p]_{A\sigma}a^{(k)+}a(\sigma) - [p]_A{}^{\sigma}a^+(\sigma)a^{(k)}\} \tag{4}$$

choosing either

$$c^{(k)}=(1,i) \quad \text{or} \quad c^{(k)}=(1,-i),$$

we get the supercharges in question, say, Q'_A and Q''_A. Notice that[5]

$$\{Q'_A,Q''^{+}_{\dot{B}}\}=m\int\frac{d^3p}{2\omega_p}p_{A\dot{B}}(a^{(1)+}+ia^{(2)+})(a^{(1)}+ia^{(2)}) \tag{5}$$

is neither proportional to $P_{A\dot{B}}$ nor equal to zero and so violates (1). Furthermore[5]

$$\{Q'_A,Q''_B\}=F_{AB}+im^2\,\epsilon_{AB}B, \tag{6}$$

where

$$F_{AB}=im^2\int\frac{d^3p}{2\omega_p}([p]_{A\sigma}[p]_B{}^{\rho}+[p]_{B\sigma}[p]_A{}^{\rho})a^+(\rho)a(\sigma)$$

$$=F_{BA}\neq 0,$$

$$B=i\int\frac{d^3p}{2\omega_p}(-a^{(1)+}a^{(2)}+a^{(2)+}a^{(1)}) \tag{7}$$

On the right-hand side of (6) one term, F_{AB}, is symmetric in the spinor indices and does not vanish; this violates, in turn, relation (2). F_{AB} is definitely not proportional[6] to M_{AB} as it commutes with P_{μ}. Of course, B also commutes with translations. Therefore Q'_A and Q''_A *cannot* be identified with, say $Q_A^{(1)}$ and $Q_A^{(2)}$, resp., appearing in relations (1), (2), and (3). This observation implies also that *at most one* of the aforementioned supercharges can coincide with the supercharge admitted by the extended Coleman–Mandula theorem in the interacting field theory.

Which of the two is the genuine supercharge and what meaning can be attributed to the other one?

This dilemma is easily solved if we take into account that the scalar free field theory is *always* covariant under the mapping

$$\varphi(x)\to -\varphi(x).$$

Let us define the unitary operator π ($\pi^2=1$) by

$$\pi a^{(1)}(\mathbf{p})\pi=a^{(1)}(\mathbf{p}),$$

$$\pi a^{(2)}(\mathbf{p})\pi=-a^{(2)}(\mathbf{p}),$$

$$\pi a(\mathbf{p},\sigma)\pi=a(\mathbf{p},\sigma);$$

then

$$Q''_A=\pi Q'_A\pi, \tag{8}$$

and vice versa. If Q'_A is the supercharge linked to the *interacting* field theory, Q''_A is not, but it is, of course—because of (8)—a good supersymmetry generator of the asymptotic free fields.

By this simple example one sees that there if *no way* to tell which of the two supercharges is the genuine one, as they are subject to changes under transformations, like π, which on the other hand do not affect the tensorial charges P_{μ}, $M_{\mu\nu}$, and B. We have to choose one of the supercharges as the genuine one and nothing goes wrong as long as we stick consistently to this choice. Similar situation arises in more complicated cases.

3. DEMOCRACY OF THE DISCRETE SYMMETRIES

The considerations presented in Sec. 2 have also another aspect which we are going to exhibit in this

section. This different feature concerns the compatibility of the π-transformation and supersymmetry in an interacting field theory.

The conclusion drawn from these considerations is as follows: in a supersymmetric model consisting of one neutral spinor field $\psi_{\text{int},A}$ and two real scalar $\varphi^{(i)}_{\text{int}}$, $i=1,2$, which *interact* with each other, the mapping

$$\psi_{\text{int},A}(x) \to \psi_{\text{int},A}(x) ,$$

$$\varphi^{(1)}_{\text{int}}(x) \to \varphi^{(1)}_{\text{int}}(x) ,$$

$$\varphi^{(2)}_{\text{int}}(x) \to -\varphi^{(2)}_{\text{int}} ,$$

cannot be a symmetry of this model.

To prove this assertion, assume on the contrary that the mapping is implemented by a unitary operator π; then, in addition to the supercharge Q'_A responsible for the supersymmetry, we would have another supercharge Q_A given by (8)[7] as well, but this would violate (1) and (2), as was shown earlier.

This assertion can be generalized. Let us consider a supersymmetric model of massive, interacting fields encompassing also scalar fields. Assume that this model is covariant under the mapping consisting of changing the sign of only some of the scalar fields, not all of them, and leaving the other fields invariant. This will be also valid, *a fortiori*, for the asymptotic free fields.

In terms of the asymptotic fields any supercharge Q'_A of the interacting field model can be expressed as a sesquilinear form of creation and annihilation operators of *all* fields appearing in the model; notice that if single field were missing in this expression we would never recover from it [by using Q'_A and (1)] the energy-momentum vector P_μ for the *whole* system of fields as the contribution of this missing field would be left out. As far as the scalar fields are concerned, Q'_A is a *linear* expression of these fields.

Let us write it in the form

$$Q'_A = a'_A + b_A + r_A = a_A + b_A , \tag{9}$$

where a'_A depends on the scalar fields which do not change the sign under the mapping, b_A depends on the scalar fields which change the sign and r_A is a term which does not depend on the scalar fields at all; as a'_A and r_A are not affected by the mapping we combine them in (9) to one term $a'_A + r_A \equiv a_A$.

As we assumed that there is a symmetry of the model corresponding to the aforementioned mapping, we have also beside (9) the supercharge

$$Q''_A = \pi Q'_A \pi = a_A - b_A . \tag{10}$$

The anticommutation relations between Q'_A and Q''_A must conform with (1); we have

$$\{Q'_A, Q'^{+}_{\dot B}\} = aP_{A\dot B} , \quad a \geq 0$$

$$\{Q'_A, Q''^{+}_{\dot B}\} = bP_{A\dot B} ,$$

$$\{Q''_A, Q'^{+}_{\dot B}\} = \bar b P_{A\dot B} ,$$

$$\{Q''_A, Q''^{+}_{\dot B}\} = cP_{A\dot B} , \quad c \geq 0 .$$

Taking into account (9) and (10) these relations yield

$$\{a_A, a^{+}_{\dot B}\} = (a + c + b + \bar b)P_{A\dot B} , \tag{11}$$

$$\{b_A, b^{+}_{\dot B}\} = (a + c - b - \bar b)P_{A\dot B} . \tag{12}$$

As the left-hand side of (11) does not depend on the scalar fields which change the sign under the mapping and the left-hand side of (12) does not depend on the scalar fields which do not change the sign, the right-hand sides of (11) and (12) *cannot* be proportional to the *whole* energy-momentum vector, unless

$$a + c = 0, \quad b + \bar b = 0$$

or—because of the nonnegativity of the matrix—

$$a = c = b = 0 ,$$

which in turn entails

$$Q'_A = Q''_A = 0, \quad A = 1, 2.$$

We conclude that in the model described above the simultaneous existence of *supersymmetry* and symmetry consisting of changing sign of only a some of scalar fields is *incompatible*.

Notice that this mapping is nevertheless a good candidate for symmetry of a model in the *absence* of supersymmetry as it does not contradict any fundamental assumption.

4. DEMOCRACY OF THE INTERNAL SYMMETRIES

An observation similar to that investigated in Sec. 3 but concerning internal symmetry will be the subject of this secion. We shall show that the presence of *supersymmetric* covariance imposes *restrictions* in the choice of the internal symmetries. To demonstrate this we shall expoit mainly the relation (3). It can easily happen that in a supersymmetric theory a generator of an internal symmetry—let us call it B—whose presence in a theory without supersymmetry is perfectly acceptable, does not conform with the basic relations and must be ruled out; e.g., we expect for every supercharge Q_A that, according to (3),

$$[Q_A, B] = \hat Q_A \neq 0$$

is a linear combination of supercharges appearing in the model, but this does not need to be the case; moreover, it may happen that

$$\{\hat Q_A, \hat Q^{+}_{\dot B}\} = V_{A\dot B} \neq \lambda P_{A\dot B} .$$

Thus $\hat Q_A \neq \Sigma s^M Q^{(M)}_A$ as well as $V_{A\dot B} \neq \lambda P_{A\dot B}$ would exclude B as a possible candidate for a generator of internal symmetry for the *interacting* theory; however, both quantities, $\hat Q_A$ and $V_{A\dot B}$, are not ruled out in an asymptotic *free* field theory, where they appear as

legitimate symmetry generators.

To make things clearer let us consider first a model consisting of *one* neutral spinor field $\psi_{\rm int}$ and two real scalar fields $\varphi^{(1)}_{\rm int}$ and $\varphi^{(2)}_{\rm int}$ interacting with each other. Let us further assume that these two real scalar fields are covariant under a U(1) transformation[8] generated by $B = B^+$ given by (7); for the asymptotic free (incoming or outgoing) fields ψ and $\varphi^{(k)}$, $k = 1, 2$ we have

$$i[B, \varphi^{(1)} + i\varphi^{(2)}] = \varphi^{(1)} + i\varphi^{(2)} ,$$
$$[B, \psi] = 0 . \tag{13}$$

Using (4) and (7) an easy computation yields

$$[Q_A, B] = \mp Q_A \tag{14}$$

for $c^{(1)} = \mp ic^{(2)} = 1$, resp. We infer from (14) that B is an *admissible* internal symmetry for an *iteracting* supersymmetrical model.

Consider, however, the case of *two* neutral spinor fields $\psi^{(a)}$, $a = 1, 2$, and *four* real scalar fields $\varphi^{(k)}$, $k = 1, 2, 3, 4$, and assume that $\varphi^{(1)}$ and $\varphi^{(2)}$ are covariant under a U(1) transformation, other fields being invariant under it,[8] i.e., we have relation (13) and

$$[B, \varphi^{(3)}] = [B, \varphi^{(4)}] = [B, \psi^{(a)}] = 0. \quad a = 1, 2 .$$

In this model we have two supercharges ($L = 1, 2$)

$$Q^{(L)}_A = \frac{im}{\sqrt{2}} \int \frac{d^3p}{2\omega_p} \sum_{k=1}^{4} \sum_{b=1}^{2} c^{(Lbk)} \sum_{\sigma=1}^{2} \{ i[p]_{A\sigma} a^{(k)+}(\sigma) a^{(b)}(\sigma)$$
$$- [p]_A{}^{\sigma} a^{(b)+}(\sigma) a^{(k)} \} ,$$

where the coefficients $c^{[Lbk]}$ have to satisfy the relations[9]

$$\sum_{a=1}^{2} c^{(La)} \bar{c}^{(Maj)} + c^{(Laj)} \bar{c}^{(Mai)} = 2\delta^{LM}\delta^{ij} , \tag{15}$$

$$\sum_{j=1}^{4} \bar{c}^{(Laj)} c^{(Mbj)} = 2\delta^{LM}\delta^{ab} , \tag{16}$$

$$\sum_{j=1}^{4} c^{(Laj)} c^{(Lbj)} = 0 . \tag{17}$$

A straightforward computation shows that

$$[Q^{(L)}_A, B]$$
$$= -\frac{m}{\sqrt{2}} \int \frac{d^3p}{2\omega_p} \sum_{i} \sum_{b} \sum_{\sigma} (i[p]_{A\sigma} a^{(b)}(\sigma) a^{(i)+} - [p]_A{}^{\sigma} a^{(b)+}(\sigma) a^{(i)}$$
$$\times (c^{(Lb4)}\delta^{i3} - c^{(Lb3)}\delta^{i4}) .$$

Here B is given by (7). If we require that the right-hand side be equal to

$$\sum_{M} s^{LM} Q^{(M)}_A ,$$

in accordance with (3), we get the relation

$$-c^{(Lb4)}\delta^{i3} + c^{(Lb3)}\delta^{i4} = is^{LM} c^{Mbi}, \tag{18}$$

which, because of (15), yields for $l = 1, 2$

$$s^{LM} = 0 ;$$

then from (18) it follows in turn that

$$c^{(Lb4)} = c^{(Lb3)} = 0 ,$$

which contradicts relations (15)–(17). Hence we conclude that in this particular model the gauge transformation U(1) which transforms *only two* of the four scalar fields, is prohibited as an internal symmetry of the interacting fields.[10] It is easy to see that a gauge transformation which simultaneously transforms $(\varphi^{(1)}, \varphi^{(2)})$ and $(\varphi^{(3)}, \varphi^{(4)})$ pairwise (which means that we have to do with two charged scalar fields) is already a good candidate for an internal symmetry of the interacting, supersymmetrical field theory.

In the two examples presented above we tried to make plausible the conjecture that the presence of supersymmetry in a model suppresses those representations of the internal symmetries which single out a certain fraction of the fields of the same spin (in the examples at hand these are the scalar fields) and favors those which encompass all of the fields of the same spin. This is what we would call *democracy* of internal symmetries in supersymmetric models.

To corroborate this conjecture we are going to present arguments relying on more general basis.

Let us consider a supersymmetric model consisting of massive scalar and spinor fields which interact with each other. Assume that this model is covariant under an internal symmetry and that the scalar fields can be separated into two sets, the fields $\{\varphi^{(j)}_{\rm int,I},\ j = 1, \ldots n_I\}$ of the first set are not affected by these symmetry transformations, while the fields of the other set $\{\varphi^{(k)}_{\rm int,II}, k = 1, \ldots, n_{\rm II}\}$ transform nontrivially. The spinor fields are invariant under these transformations. The same will be true for the incoming and outgoing free fields $\{\varphi_{\rm I}\}$, $\{\varphi_{\rm II}\}$, etc. Let us concentrate on the action of one of the generators of these internal group transformations which we shall call B. For the free asymptotic fields we have

$$[B,\ \varphi^{(j)}_{\rm I}] = 0,\ j = 1, \ldots, n_{\rm I} , \tag{19}$$
$$[B, \varphi^{(k)}_{\rm II}] = \sum_{j=1}^{n_{\rm I}} a^{kj} \varphi^{(j)}_{\rm I} + \sum_{l=1}^{n_{\rm II}} b^{kl} \varphi^{(l)}_{\rm II},\quad k = 1 \ldots n_{\rm II} . \tag{20a}$$

From the Jacobi identity of $(B,\ \varphi^{(k)}_{\rm II}, \varphi^{(m)}_{\rm I})$ it follows that

$$a^{km} = 0 . \tag{20b}$$

As was mentioned earlier in Sec. 3, every spinorial charge Q_A is a linear form of *all* the scalar field appearing in the model, viz.,

$$Q_A = \sum_{j=1}^{n_{\rm I}} \alpha^j_A(\varphi^{(j)}_{\rm I}) + \sum_{k=1}^{n_{\rm II}} \beta^k_A(\varphi^{(k)}_{\rm II}) .$$

As B does commute with $\varphi_{\rm I}$ and spinorial fields we have by virtue of (19) and (20)

$$[B, Q_A] = \sum_{k=1}^{n_{\rm II}} [B, \beta^k_A(\varphi^k_{\rm II})]$$
$$= \sum_{k=1}^{n_{\rm II}} \sum_{l=1}^{n_{\rm II}} b^{kl} \beta^k_A(\varphi^l_{\rm II}) = Q'_A .$$

As Q'_A does not depend on the fields φ^I_I, $\{Q'_A, Q'^*_B\}$ cannot be proportional to $P_{A\dot{B}}$, the latter representing the energy momentum vector of the *whole* system including also φ_I, *unless* $Q'_A=0$. $Q'_A\neq 0$ can not be a linear combination of spinorial charges inherent in the model, as required by (3); these charges conform namely, with (1). The *only* solution is $Q'_A=0$, which leads to the relation among b^{kl} and coefficients in front of φ in $\beta^k_A(\varphi)$ summed over k; this seems to be a rather special case, which needs further investigation.

A similar reasoning can be applied in the case when the roles of scalar and spinor fields are interchanged.

The conclusion resulting from these consideration reads: an internal symmetry which transforms only a *part* of fields of a fixed spin, leaving the other fields unaffected, and does not commute with *all* supercharges *cannot be* admited as a symmetry in an interacting *supersymmetric* field theory, although it can be a *good* internal symmetry in the absence of supersymmetric covariance.

This statement can be further generalized, say, to the case of supersymmetric quantum theory of scalar, spinor, *and* vector fields.

Each supercharge

$$Q_A=\sum_{i=1}^{s} Q^{(i)}_{S,A}(\varphi^{(i)})+\sum_{z=1}^{v} Q^{(z)}_{V,A}\,V^{(z)}$$

is a linear functional in all the asymptotic scalar real fields $\varphi^{(i)}$, $i=1, \ldots, s$, and Hermitian vector fields $V^{(z)}_{A\dot{B}}$, $z=1, \ldots, v$ (all of them of the same mass).

Assume now that under an internal symmetry induced by some generators B_l, $l=1, \ldots, n$, only the scalar free fields are linearly transformed while the spinor and vector fields remain unaffected. Then for each B_l, which we shall call B,

$$[B,Q_A]=Q'_A=\sum_{i=1}^{s} Q'^{(i)}_{S,A}(\varphi^{(i)})$$

no longer depends on $V^{(z)}$ and therefore $\{Q'_A, Q'^*_B\}$ cannot reproduce the *whole* energy-momentum vector of the fields involved *unless* $Q'_A=0$. For $Q'_A\neq 0$ the extended Coleman–Mandula Theorem is violated.

To summarize, let us state the following assertion about the *democracy of internal symmetries in supersymmetrical quantum field theories*: an internal symmetry which transforms only some fields of a fixed spin, leaving the other fields unaffected and which acts nontrivially on *at least one* supercharge, *cannot be* admitted as a symmetry in an interacting *supersymmetric* field theory, although it can be a *good* internal symmetry in the absence of supersymmetric covariance; moreover, in the case of a model consisting of scalar, spinor, and vector fields even a symmetry which transforms all of the scalar (vector) fields leaving spinor and vector (scalar) fields unaffected is also ruled out.

ACKNOWLEDGMENTS

The author is grateful to Professor R. Haag, Professor J. Lukierski, and Mr. M. Wolf for discussion and critical remarks.

[1]R. Haag, J. T. Łopuszański, and M. Sohnius, Nucl. Phys. B **88**, 257 (1975).
[2]S. Coleman and T. Mandula, Phys. Rev. **159**, 1251 (1967); J. T. Łopuszański, J. Math. Phys. **12**, 2401 (1971).
[3]Should c^{LM} be a nonnegative Hermitian matrix, the spinorial charges would be linearly dependent, as from (1) it follows that

$$\tfrac{1}{2}(\psi,\{Q^f_1,Q^{f*}_1\}\psi)+\tfrac{1}{2}(\psi,\{Q^f_2,Q^{f*}_2\}\psi)$$
$$=\sum_L\sum_M f^L\bar{f}^M c^{LM}(\psi,P_0\psi),$$

with

$$\sum f^L Q^{(L)}_A\equiv Q^f_A$$

for every Hilbert state ψ from the domain of definition.
[4]We know from other fundamental considerations that these groups have to be compact. See, e.g., S. Doplicher, R. Haag, and J. Roberts, Commun. Math. Phys. **23**, 199 (1971); **35**, 49 (1974).
[5]It is advisable for computation purposes to remember that $[p]_B{}^D=([p]\epsilon[p]^T)_{AB}=\epsilon_{AB}$ and $\sum_C[p]_A{}^C[\bar{p}]_B{}^C=\frac{1}{m}(\sigma^\mu)_{A\dot{B}}p_\mu=\frac{1}{m}p_{A\dot{B}}$, as for $A\epsilon SL(2,C)$ we have $(A^{-1})_A{}^B=-A_A{}^B$.
[6]$M_{AB}=M_{BA}$ are three generators of the SU(2) subgroup of the Lorentz group defined as follows:

$$M_{AB}=\tfrac{1}{2}(\sigma^u)_{A\dot{C}}(\sigma^v)_B{}^{\dot{C}}M_{\mu\nu}.$$

[7]Notice that the generators of (super) symmetries of the *interacting* fields are *global* quantities and, as such, are identical with those for the asymptotic free fields.
[8]The Coleman-Mandula Theorem definitely does not prevent such a transformation.
[9]J. T. Łopuszański, Rep. Math. Phys. **9**, 301 (1976).
[10]Of course, it is a good symmetry for the asymptotic *free* field theory.

On a new Bose–Fermi mixing symmetry

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(Received 8 May 1981; accepted for publication 1 August 1981)

The Bose–Fermi symmetry manifest in supersymmetry has non-super-symmetric realizations. Two examples of a new Bose–Fermi symmetry, called Clifford symmetry, are discussed. In the first example, the spin content of the Clifford multiplet (the analog of a supersymmetry particle multiplet) is $4(0,0) + 2\{(\frac{1}{2},0) + (0,\frac{1}{2})\} + (\frac{1}{2},\frac{1}{2})$; in the second example it is $25(0,0) + 20\{(\frac{1}{2},0) + (0,\frac{1}{2})\} + 5\{(1,0) + (0,1)\} + 16(\frac{1}{2},\frac{1}{2}) + 4\{(1,\frac{1}{2}) + (\frac{1}{2},1)\} + (1,1)$. The mass matrix for a Clifford multiplet is, in general, not a multiple of the unit matrix (which it is, however, required to be for an irreducible supersymmetry particle multiplet).

PACS numbers: 11.30.Pb, 02.20. + b

I. INTRODUCTION

The (extended) supersymmetry algebra is a nontrivial graded extension of the Lie algebra of the Poincaré group.[1,2] As with the Poincaré group, the irreducible representations of the supersymmetry group fall into classes according to whether the momentum is timelike, lightlike, spacelike, or zero. Supersymmetry particle multiplets have been constructed by means of the Wigner–Mackey method of induced representations[3]; these states are labeled according to the value of p_α of the momentum, and by the eigenvalues of a complete set of commuting operators associated with the little group of p_α. In particular, in the case of timelike momenta, $p^2 = -m^2$, a supersymmetry particle multiplet with the spin content $(m, j-\frac{1}{2}) + 2(m,j) + (m, j+\frac{1}{2})$ exists for each $j = 0,\frac{1}{2},1,\ldots$ and for each value of $m > 0$. The cases $j = 0,\frac{1}{2}$ are the well-known chiral and vector particle multiplets, respectively.

Speaking very loosely, there is another way, completely different from supersymmetry, to generate particle multiplets that contain both bosons and fermions. The idea is very simple. When one takes the "square root" of the Klein–Gordon equation to produce the Dirac equation, spinor representations of O(3,1) and spin $-\frac{1}{2}$ appear. If one then takes the square root of the Dirac equations, not spin $-\frac{1}{4}$ objects [SU(2) is simply connected!], but geometrical objects that contain spin $0,\frac{1}{2}$, and $1 = j_{\max}$ arise in the formalism. Take the square root again, and geometrical objects containing spin $0,\frac{1}{2},1,\frac{3}{2}$, and $2 = j_{\max}$ appear; and so on. In each case, the geometrical objects that arise in the formalism are rank-one tensors that transform under a certain pseudo-orthogonal group containing $\overline{\mathrm{O}(3,1)}$, whose representation is generated by a set of elements in the enveloping algebra of an irreducible representation of a Clifford algebra C. Upon restriction to the $\overline{\mathrm{O}(3,1)}$ subgroup, these tensors decompose into the direct sum of irreducible $\overline{\mathrm{O}(3,1)}$ representations. The dimensions and spin content of these tensors is fixed. This is clearly not equivalent to what happens in supersymmetry, where, for example in the timelike momentum class, unitary irreducible representations exist for each value of j, of dimension $4(2j+1)$.[3] Yet in both formalisms symmetry transformations exist that mix bosons and fermions. In the present case the symmetry transformations are given by $\exp\{E\}$, where E generates C. It seems appropriate to name this new symmetry *Clifford symmetry*, after W. K. Clifford.

In this paper the two simplest representations of Clifford transformations are considered, namely the representation associated with $j_{\max} = 1$ in which $C = C_8$, and the representations associated with $j_{\max} = 2$ in which $C = C_{16}$. For these cases, denoting the rank-one Clifford tensor by ϕ, the $\overline{\mathrm{O}(3,1)}$ decomposition is (i) ($j_{\max} = 1$; dim $\phi = 16$) $\phi = 4(0,0) + 2\{(\frac{1}{2},0) + (0,\frac{1}{2})\} + (\frac{1}{2},\frac{1}{2})$; and (ii) ($j_{\max} = 2$; dim $\phi = 256$) $\phi = 25(0,0) + 20\{(\frac{1}{2},0) + (0,\frac{1}{2})\} + 5\{(1,0) + (0,1)\} + 16(\frac{1}{2},\frac{1}{2}) + 4\{(1,\frac{1}{2}) + (\frac{1}{2},1)\} + (1,1)$.

II. BASIC FORMALISM

The lowest-dimension Clifford multiplet is formed from a 16-component irreducible $\overline{\mathrm{O}(4,4)}$ spinor which under the restriction of $\overline{\mathrm{O}(4,4)}$ to an $\overline{\mathrm{O}(3,1)}$ subgroup, decomposes into the direct sum $4(0,0) + 2\{(\frac{1}{2},0) + (0,\frac{1}{2})\} + (\frac{1}{2},\frac{1}{2})$. The restriction of $\overline{\mathrm{O}(4,4)}$ to $\overline{\mathrm{O}(3,1)}$ is realized as follows:

Let γ^α ($\alpha,\beta,\cdots = 1,2,3,4$) denote a real 4×4 irreducible (Majorana) representation of the Dirac matrices, where

$$\gamma^\alpha\gamma^\beta + \gamma^\beta\gamma^\alpha = 2g^{\alpha\beta} \tag{1}$$

and

$$g_{\alpha\beta} = g^{\alpha\beta} = \mathrm{diag}(1,1,1,-1). \tag{2}$$

Define

$$\gamma^5 = -\frac{1}{4!}\epsilon_{\alpha\beta\mu\nu}\gamma^\alpha\gamma^\beta\gamma^\mu\gamma^\nu = -\gamma^1\gamma^2\gamma^3\gamma^4, \tag{3}$$

and

$$\epsilon = \gamma^4\gamma^5 \tag{4}$$

(note that ϵ, γ^4, and γ^5 are skew symmetric and have square equal to -1). The antisymmetrized products of the γ^α

$$S^{\alpha\beta} = -\tfrac{1}{4}[\gamma^\alpha,\gamma^\beta], \tag{5}$$

satisfy

$$[S^{\alpha\beta},\gamma_\mu] = \delta^\alpha_\mu\gamma^\beta - \delta^\beta_\mu\gamma^\alpha \tag{6}$$

 0022-2488/81/122957-04$01.00

and

$$[S^{\alpha\beta},S^{\mu\nu}] = g^{\alpha\mu}S^{\beta\nu} - g^{\alpha\nu}S^{\beta\mu} - g^{\beta\mu}S^{\alpha\nu} + g^{\beta\nu}S^{\alpha\mu}, \quad (7)$$

and are the generators of a four-dimensional irreducible representation of $\overline{\mathrm{SO}(3,1)}$;

$$S^{\alpha\beta} \to \exp\left[\tfrac{1}{2}\omega_{\alpha\beta}S^{\alpha\beta}\right] = S \in \overline{\mathrm{SO}(3,1)}, \quad (8)$$

where the $\omega_{\alpha\beta} = -\omega_{\beta\alpha}$ are six real parameters. (For notational simplicity, throughout this paper a representation of a group G is simply denoted as G.) Since (tilde denotes transpose)

$$\tilde{\gamma}^{\alpha}\gamma^{A} = -\gamma^{A}\gamma^{\alpha} \quad (9)$$

and

$$\tilde{\gamma}^{\alpha}\epsilon = \epsilon\gamma^{\alpha}, \quad (10)$$

one finds that

$$\tilde{S}^{\alpha\beta}\gamma^{A} = -\gamma^{A}S^{\alpha\beta} \quad (11)$$

and

$$\tilde{S}^{\alpha\beta}\epsilon = -\epsilon S^{\alpha\beta}, \quad (12)$$

so that, for $S \in \overline{\mathrm{SO}(3,1)}$,

$$\tilde{S}\gamma^{A} = \gamma^{A}S^{-1} \quad (13)$$

and

$$\tilde{S}\epsilon = \epsilon S^{-1}. \quad (14)$$

Equations (13) and (14) may be written as $\rho = \tilde{S}\rho S$, with ρ equal to ϵ or γ^{A}. ρ is skew symmetric; if, however, there exists a symmetric matrix $\tau = \tilde{\tau} \leftrightarrow \tau_{qp} = \tau_{pq}$ that satisfies $\tau = \tilde{S}\tau S$, then one can define a set of matrices E_q by $E_qE_p + E_pE_q = 2\tau_{qp}$, and generate particle states that transform under the group generated by a set of elements in the enveloping algebra of the E_q. This is a mechanism whereby one can generate particle multiplets containing both bosons and fermions. Since $\tilde{\rho} = -\rho$, ρ cannot be utilized in this construction. However, by Eq. (9), $\gamma^{A}\gamma^{\alpha}p_{\alpha}$ is symmetric, and moreover satisfies an equation of the form $\gamma^{A}\gamma^{\alpha}p_{\alpha} = \tilde{S}\gamma^{A}\gamma^{\alpha}p'_{\alpha}S$ [where $p'_{\alpha} = \Lambda_{\alpha}{}^{\beta}p_{\beta}$, and $\Lambda \in \mathrm{SO}(3,1)$], since

$$\gamma^{\alpha} = \Lambda^{\alpha}{}_{\beta}S\gamma^{\beta}S^{-1} \quad (15)$$

under SO(3,1). [Here $\Lambda^{\alpha}{}_{\beta} = \delta^{\alpha}_{\beta} - \omega^{\alpha}{}_{\beta} + \cdots = (e^{-\omega})^{\alpha}{}_{\beta}$.] Therefore a set of operators E_q may be defined by $E_qE_p + E_pE_q = 2(\gamma^{A}\gamma^{\alpha}p_{\alpha})_{qp}$, $[p_{\alpha},E_q] = 0$, and $[J^{\alpha\beta},E_q] = iS^{\alpha\beta}_{qp}E_p$, thereby realizing a grading of the Poincaré Lie algebra and supersymmetry.[21]

If one wants to construct a p_{α}-independent symmetric matrix τ satisfying an equation similar to $\tau = \tilde{S}\tau S$, then one must utilize a group larger than $\overline{\mathrm{O}(3,1)}$. We shall utilize $\overline{\mathrm{O}(3,3)}$. Let Γ^{A} ($A,B,\ldots, = 1,\ldots,6$) be six real matrices that generate an irreducible representation of the Clifford algebra C_6

$$\Gamma^{A}\Gamma^{B} + \Gamma^{B}\Gamma^{A} = 2g^{AB}, \quad (16)$$

where

$$g_{AB} = g^{AB} = \mathrm{diag}(1,1,1,-1,-1,-1). \quad (17)$$

Define

$$\Gamma^{7} = \frac{1}{6!}\epsilon_{ABCDEF}\Gamma^{A}\Gamma^{B}\Gamma^{C}\Gamma^{D}\Gamma^{E}\Gamma^{F}; \quad (18)$$

then

$$\Gamma^{A}\Gamma^{7} + \Gamma^{7}\Gamma^{A} = 0 \quad (19)$$

and

$$(\Gamma^{7})^{2} = 1. \quad (20)$$

A particular representation of the Γ matrices is

$$\Gamma^{\alpha} = \begin{pmatrix} 0 & \gamma^{\alpha}\epsilon \\ -\epsilon\gamma^{\alpha} & 0 \end{pmatrix}, \quad (21)$$

$$\Gamma^{5} = \begin{pmatrix} 0 & \gamma^{5}\epsilon \\ -\epsilon\gamma^{5} & 0 \end{pmatrix}, \quad (22)$$

$$\Gamma^{6} = \begin{pmatrix} 0 & -\epsilon \\ -\epsilon & 0 \end{pmatrix}, \quad (23)$$

and

$$\Gamma^{7} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (24)$$

The generators of $\overline{\mathrm{SO}(3,3)}$ are

$$M^{AB} = -\tfrac{1}{4}[\Gamma^{A},\Gamma^{B}], \quad (25)$$

and they satisfy

$$[M^{AB},\Gamma_{R}] = \delta^{A}_{R}\Gamma^{B} - \delta^{B}_{R}\Gamma^{A} \quad (26)$$

and

$$[M^{AB},M^{RS}] = g^{AR}M^{BS} - g^{AS}M^{BR} - g^{BR}M^{AS} + g^{BS}M^{AR}. \quad (27)$$

In the particular representation of Eqs. (21)–(24), the $M^{\alpha\beta}$ are given by

$$M^{\alpha\beta} = \begin{pmatrix} S^{\alpha\beta} & 0 \\ 0 & -\tilde{S}^{\alpha\beta} \end{pmatrix} \quad (28)$$

and M^{56} is represented as

$$M^{56} = -\frac{1}{2}\begin{pmatrix} \gamma^{5} & 0 \\ 0 & \gamma^{5} \end{pmatrix}. \quad (29)$$

An element $M \in \overline{\mathrm{SO}(3,1)}$ is given by

$$M = \begin{pmatrix} S & 0 \\ 0 & \tilde{S}^{-1} \end{pmatrix}, \quad (30)$$

where S is defined in Eq. (8).

In order to construct the symmetric τ matrix, we must first define a rank-two antisymmetric $\overline{\mathrm{O}(3,3)}$ "metric," denoted as Ω. Ω may be defined by requiring that

$$\tilde{\Gamma}^{A}\Omega = \Omega\Gamma^{A}. \quad (31)$$

Then

$$\tilde{\Gamma}^{7}\Omega = -\Omega\Gamma^{7} \quad (32)$$

and

$$\tilde{M}^{AB}\Omega = -\Omega M^{AB}, \quad (33)$$

so that

$$\Omega = \tilde{M}\Omega M \quad (34)$$

for $M \in \overline{\mathrm{SO}(3,3)}$. In the above representation, Ω may be cho-

sen to be

$$\Omega = \Gamma^1\Gamma^2\Gamma^3 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{35}$$

There are two possible choices for a p_α-independent symmetric matrix τ satisfying $\tau = \tilde{M}\tau M$, $M \in$ SO(3,1). The first is $\tau = -\Omega\Gamma^7 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ [in this case, $\tau = \tilde{M}\tau M$ is valid for $M \in$ SO(3,3)], and the second choice is $\tau = -\Gamma^4\Gamma^7 = 2\Omega M^{56} = \begin{pmatrix} 0 & -\gamma^5 \\ \gamma^5 & 0 \end{pmatrix}$. The choice for τ is contingent on the following observation. The parity transformation ($x^i \to -x^i$, $t \to t$) contained in O(3,3) may be represented by $M_P = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, and the time-reversal transformation ($x^i \to x^i$, $t \to -t$) represented by $M_T = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$.[4] Now $\tilde{M}_P\Omega\Gamma^7 M_P = \Omega\Gamma^7$ and $\tilde{M}_T\Omega\Gamma^7 M_T = -\Omega\Gamma^7$, while $\tilde{M}_P 2\Omega M^{56} M_P = -2\Omega M^{56}$ and $\tilde{M}_T 2\Omega M^{56} M_T = 2\Omega M^{56}$. Thus it is possible to formulate this representation of Clifford symmetry in a manner that retains one of the discrete symmetries of parity or time reversal as a manifest symmetry, but not both. We shall retain time reversal as a manifest symmetry, and therefore we define

$$\tau = 2\Omega M^{56}. \tag{36}$$

At this point we must introduce some index notation. Let ψ denote an O(3,3) spinor that transforms under the 8×8 irreducible representation of O(3,3) that has been defined above. Associate O(3,3), indices as follows: $\psi \leftrightarrow \psi^a$ ($a,b,\ldots = 1,\ldots,8$) $\Omega \leftrightarrow \Omega_{ab} = -\Omega_{ba}$; $\tilde{\psi}\Omega \leftrightarrow \psi_b = \psi^a\Omega_{ab}$; $-\Omega^{-1} \leftrightarrow \Omega^{ab}$, and so the convention is $\Omega^{ab}\Omega_{bc} = -\delta^a_c$. According to this convention, spinor indices are to be raised according to $\psi^a = \Omega^{ab}\psi_b$ and lowered according to $\psi_b = \psi^a\Omega_{ab}$; $\Gamma^A \leftrightarrow \Gamma^{Aa}{}_b$. In index notation Eq. (31) reads $\Gamma^A_{ab} = -\Gamma^A_{ba}$, Eq. (32) as $\Gamma^7_{ab} = \Gamma^7_{ba}$, Eq. (33) as $M^{AB}_{ab} = M^{AB}_{ba}$, and Eq. (34) as $\Omega_{ab} = M^c{}_a\Omega_{cd}M^d{}_b$. Equation (36) is $\tau_{ab} = 2\Omega_{ac}M^{56c}{}_b = -2M^{56}_{ab}$.

We are now equipped to formulate the main result of this paper. Let E_a denote the generators of a real irreducible representation of the 2^8-dimensional (pseudo -) Clifford algebra C_8. The E_a are required to be real and to satisfy

$$E_aE_b + E_bE_a = 2\tau_{ab}. \tag{37}$$

The 2^8 antisymmetrized products of the E_a comprise a basis for C_8, and the E_a may be represented by real $2^{8/2}\times 2^{8/2}$ matrices. The E_a are related to e_a satisfying

$$e_ae_b + e_be_a = 2g_{ab}, \tag{38}$$

$$g_{ab} = \text{diag}(1,1,1,1,-1,-1,-1,-1), \tag{39}$$

by an orthogonal transformation $E_a = e_bT^b{}_a$, where

$$T = -\sqrt{2}\begin{pmatrix} S^{34} & S^{12} \\ S^{12} & S^{34} \end{pmatrix}.$$

The $e_{ab} = -\frac{1}{4}[e_a,e_b]$, and hence the

$$E_{ab} = -\tfrac{1}{4}[E_a,E_b] \tag{40}$$

generate a (real) irreducible 16×16 dimensional representation of O(4,4). The E_{ab} satisfy

$$[E_{ab},E_c] = \tau_{ac}E_b - \tau_{bc}E_a \tag{41}$$

and

$$[E_{ab},E_{cd}] = \tau_{ac}E_{bd} - \tau_{ad}E_{bc} - \tau_{bc}E_{ad} + \tau_{bd}E_{ac}. \tag{42}$$

We recall that $\tau = \tilde{M}\tau M$ for $M \in$ SO(3,1) and $M = M_T$. This may also be expressed as

$$\tau_{ab} = M^c{}_a\tau_{cd}M^d{}_b. \tag{43}$$

Consider the matrices $E_aM^a{}_b$; they satisfy the same anticommutation relations as the E_a: $E_cM^c{}_aE_dM^d{}_b + E_dM^d{}_bE_cM^c{}_a = 2M^c{}_a\tau_{cd}M^d{}_b = 2\tau_{ab}$. Therefore the $E_aM^a{}_b$ generate an irreducible representation of C_8. However there is only one irreducible representation of C_n for n even.[5] Thus the $E_aM^a{}_b$ are isomorphic to the E_a, i.e., there exists an $L \in$ {the restriction of O(4,4) to an O(3,1) subgroup} such that

$$E_bM^b{}_a = L^{-1}E_aL. \tag{44}$$

Therefore there exists a 2-1 map of the representation of { O(4,4) restricted to O(3,1) } generated by the E_{ab} into the representation of O(3,1) generated by the $M^{\alpha\beta}$, which is given by

$$M^b{}_a = \frac{\tau^{bc}}{16}\,\text{tr}L^{-1}E_aLE_c. \tag{45}$$

The map is into and not onto because, for example, as we have seen above, the parity transformation M_p does not preserve τ [in the sense of Eq. (43)], so that $L(M_p)$ does not exist, [Note that $L(\tilde{R}M_pR)$ exists, where R is an automorphism that maps τ into $\Omega\Gamma^7$: $\tau \to \Omega\Gamma^7 = R\tau\tilde{R}$, $\tilde{R} = R^{-1}$. However, $\tilde{R}M_pR$ does not represent the parity transformation.]

For $M(\omega) = \exp\{1/2\omega_{\alpha\beta}M^{\alpha\beta}\} \in$ SO(3,1), $L(\omega)$ is explicitly given by

$$L(\omega) = \exp\{1/2\theta^{ab}E_{ab}\} \in \text{SO(3,1)}, \tag{46}$$

where

$$\theta^{ab} = -\theta^{ba} = 1/2\omega_{\alpha\beta}M^{\alpha\beta a}{}_c\tau^{cb}. \tag{47}$$

This representation of SO(3,1) is, of course, reducible [as is the representation provided by the $M(\omega)$]. The form of Eqs. (46) and (47) suggests that we define the quantities

$$E^{\alpha\beta} = \tfrac{1}{2}M^{\alpha\beta a}{}_c\tau^{cb}E_{ab}, \tag{48}$$

which are the generators of a reducible representation of SO(3,1). [If one picks a representation of the E_a, then it is straightforward to construct a unitary (orthogonal) similarity transformation U that reduces the $E^{\alpha\beta}$ to the direct sum

$$U^{-1}E^{\alpha\beta}U = \begin{pmatrix} S^{\alpha\beta} & 0 & 0 & 0 \\ 0 & -\tilde{S}^{\alpha\beta} & 0 & 0 \\ 0 & 0 & -g^{\mu\lambda}\delta^{\alpha\beta}_{(\mu)(\nu)} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \tag{49}$$

$= 2\{(\frac{1}{2},0) + (0,\frac{1}{2})\} + (\frac{1}{2},\frac{1}{2}) + 4(0,0)$, where 0 in Eq. (49) represents the 4×4 zero matrix. We shall derive this spin content

again below in a different manner.]

The first example of a Clifford multiplet ϕ of (contravariant) rank one is defined to be a 16-component irreducible $\overline{\mathrm{O}(4,4)}$ spinor that transforms under $\overline{\mathrm{SO}(3,1)}$ according to

$$\phi \mapsto \phi' = L(\omega)^{-1}\phi, \tag{50}$$

where $L(\omega)$ is defined in Eq. (46), and under time reversal according to

$$\phi \mapsto \phi' = L_T{}^{-1}\phi, \tag{51}$$

where L_T satisfies Eq. (44) with $M = M_T$.

The spin content of ϕ may be derived as follows. Since ϕ has 16 components, it can be expanded in terms of the linearly independent basis vectors of a 2^4-dimensional Grassmann algebra $\mathscr{G}_4$. Let e_i $(i,j,k,h = 1,2,3,4)$ generate $\mathscr{G}_4$: $e_ie_j + e_je_i = 0$; then 1, e_i, e_ie_j $(i<j)$, $e_ie_je_k$ $(i<j<k)$, and $e_1e_2e_3e_4$ comprise a linearly independent basis for $\mathscr{G}_4$. Formally one may write $\phi = \phi_0 + \phi^i e_i + \frac{1}{2}\phi^{ij}e_ie_j + \cdots$. ϕ contains spin $-\frac{1}{2}$, so the indices $\{i,j,k,h\}$ may be identified as SL(2,$\mathbb{C}$) spinor indices. ϕ transforms in a covariant manner under time reversal, so we must have equal numbers of $(\frac{1}{2},0)$ and $(0,\frac{1}{2})$ indices. Therefore we put $e_i = (\theta_A, \theta^{X'})$ [θ_A is a two-component spinor transforming under $D^{(1/2,0)}$; $\theta^{X'}$ is a two-component spinor transforming under $D^{(0,1/2)}$], and write ϕ as $\phi = \phi_0 + \phi^A\theta_A + \phi_{X'}\theta^{X'} + \frac{1}{2}\phi^{AB}\theta_A\theta_B + \cdots$. Using the usual techniques of symmetrizing and taking traces, one finds that the SL(2,$\mathbb{C}$) decomposition of ϕ is given by $\phi = 4(0,0) + 2\{(\frac{1}{2},0) + (0,\frac{1}{2})\} + (\frac{1}{2},\frac{1}{2})$.

The set of symmetry transformations that produces the Bose–Fermi mixing in this formalism is generated by the E_a, and is an eight-anticommuting-parameter family of transformations whose generic member we denote as

$$C(\psi) = \exp\left\{\frac{1}{\sqrt{2}}E_a\psi^a\right\}, \tag{52}$$

where ψ^a is a real $\overline{\mathrm{O}(3,3)}$ spinor-valued Grassmann variable

$$\psi^a\psi^b + \psi^b\psi^a = 0. \tag{53}$$

The product of two such transformations is given by
$C(\psi_1)C(\psi_2) = \exp\{2^{-1/2}E_a\psi_1^a + 2^{-1/2}E_a\psi_2^a$
$+ \frac{1}{2}\cdot\frac{1}{2}[E_a\psi_1^a, E_b\psi_2^b] +$
$\frac{1}{12}[2^{-1/2}E_a(\psi_1^a - \psi_2^a), \frac{1}{2}[E_b\psi_1^b, E_c\psi_2^c]] + \ldots\}$
$= \exp\{1/2\tau_{ab}\psi_1^a\psi_2^b\}\, C(\psi_1 + \psi_2)$, where we have used the well-known Baker–Cambell–Hausdorff formula, and $[E_a\psi_1^a, E_b\psi_2^b] = 2\tau_{ab}\psi_1^a\psi_2^b$, along with $[\psi,\psi_1,\psi_2] = 0$. Therefore the set of $C(\psi)$ mesh together to form a type of ray representation of an abelian group.

Let $\psi'^a = M^a{}_b\psi^b$; then by Eq. (44), $E_aM^a{}_b\psi^b = E_a\psi'^a$
$= L^{-1}E_a\psi^aL$. Thus $\exp\{(2^{-1/2})E_a\psi'^a\}$
$= L^{-1}\exp\{(2^{-1/2}E_a\psi^a\}L$, or

$$C(\psi') = L^{-1}C(\psi)L. \tag{54}$$

Therefore, if $\phi' = L^{-1}\phi$ and $\bar{\phi} = C\phi$, then $\overline{(\phi')} = C'\phi' = C'L^{-1}\phi = L^{-1}C\phi = L^{-1}\bar{\phi} = (\bar{\phi})'$, so that the Clifford symmetry and Lorentz symmetry are compatible.

In order to construct an $\overline{\mathrm{O}(4,4)}$ [restricted to $\overline{\mathrm{O}(3,1)}$] scalar Langrangian from ϕ, an $\overline{\mathrm{O}(4,4)}$ rank-two metric spinor χ is needed. We define χ by requiring that

$$\tilde{E}_a\chi = -\chi E_a. \tag{55}$$

The minus sign is required in this equation so that

$$\tilde{C}\chi = \chi C^{-1}. \tag{56}$$

Equation (55) implies that

$$\tilde{E}_{ab}\chi = -\chi E_{ab}, \tag{57}$$

so that

$$\tilde{L}\chi = \chi L^{-1}, \tag{58}$$

for $L \in \overline{\mathrm{SO}(3,1)}$. Since the E_a are linearly related to the e_a, χ may be equivalently defined by $\tilde{e}_a\chi = -\chi e_a$. e_1, e_2, e_3, and e_4 are symmetric, while e_5, e_6, e_7, and e_8 are skew symmetric, so that one choice for χ is

$$\chi = e_1e_2e_3e_4. \tag{59}$$

Notice that

$$\tilde{\chi} = \chi \tag{60}$$

and

$$\chi^2 = 1. \tag{61}$$

We shall not pursue the construction of a Langrangian field theory based on this Clifford multiplet other than to point out that the mass matrix M appearing in such a theory need not be a multiple of the identity (in contrast to supersymmetry, where all of the particles in an irreducible multiplet must possess the same mass). Under a Clifford transformation C, M transforms according to

$$M \mapsto \bar{M} = CMC^{-1}, \tag{62}$$

so that a term such as $\phi^\dagger\chi M\phi$ in the Langrangian is invariant under a Clifford transformation:

$$\bar{\phi}^\dagger\chi\bar{M}\bar{\phi} = \phi^\dagger\tilde{C}\chi\bar{M}C\phi = \phi^\dagger\chi C^{-1}\bar{M}C\phi = \phi^\dagger\chi M\phi.$$

By Eq. (60), χ is symmetric: $\chi \leftrightarrow \chi_{ij} = \chi_{ji}$ $(i,j,\ldots = 1,\ldots,16)$. Therefore we can reproduce the previous calculation with χ replacing τ. Define the generators F_i of a real irreducible representation of the 2^{16}-dimensional (pseudo -) Clifford algebra C_{16} by

$$F_iF_j + F_jF_i = 2\chi_{ij}. \tag{63}$$

Then

$$F_{ij} = -\tfrac{1}{4}[F_i,F_j] \tag{64}$$

generate an (irreducible) representation of $\overline{\mathrm{O}(8,8)}$. A Clifford multiplet ϕ of dimension $2^{16/2} = 256$ can be defined to be an $\overline{\mathrm{O}(8,8)}$ [restricted to $\overline{\mathrm{O}(3,1)}$] spinor. Using an argument analogous to the discussion following Eq. (51), the spin content of ϕ may be evaluated by expanding ϕ in terms of four spinor-valued Grassmann variables $(\theta_A, \theta^{X'}; \zeta_A, \zeta^{X'})$. One finds that the SL(2,$\mathbb{C}$) content of ϕ is given by $\phi = 25(0,0) + 20\{(\frac{1}{2},0) + (0,\frac{1}{2})\} + 5\{(1,0) + (0,1)\} +$ $16(\frac{1}{2},\frac{1}{2}) + 4\{(1,\frac{1}{2}) + (\frac{1}{2},1)\} + (1,1)$. As with the previous Clifford multiplet, the mass matrix for this ϕ need not be a multiple of the identity matrix. If one requires the mass matrix M to be Lorentz invariant, $M = L^{-1}ML$, then M is only required to be a multiple of the identity on each irreducible SL(2,$\mathbb{C}$) subspace.

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A statistical approach to perturbation theory and inverse-energy-weighted sum rules [a)]

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(Received 18 April 1980; accepted for publication 20 July 1981)

A distribution function formalism is developed for perturbation theory and inverse-energy-weighted sum rules (IEWSR). The second-order perturbation is linear in the CLT (central limit theorem) limit. A polynomial expansion is also developed for the same. Finally, some applications are indicated.

PACS numbers: 21.60. – n

1. INTRODUCTION

A statistical approach to nuclear structure calculations known as the spectral distributions method or statistical spectroscopy has been recently developed,[1] in part, to overcome a major practical limitation in the conventional shell-model[2] approach. By dispensing with the need to know the nuclear wavefunctions these statistical methods make it possible to handle calculations in large model spaces. The theory is based on the recognition of certain simplifying features arising out of the many-particle nature of the model spaces, by virtue of which, strengths and expectation values exhibit, in most cases, a smooth behavior (with small fluctuations) over the model space spectrum. Recently, the method was successfully applied to the study of electromagnetic sum-rules,[3] beta-decay giant resonances,[4] single-nucleon transfer,[5] and so on. In this paper we extend[3] this statistical approach to perturbation theory and inverse-energy-weighted sum-rules.

In a conventional nuclear shell-model[2] calculation, one first generates the eigenvalue and eigenvectors of the Hamiltonian in a many-particle model space consisting of m particles distributed among N single-particle states with two-body interactions between the particles. Then the expectation values and strength functions of other operators of interest are calculated in the Hamiltonian eigenstates. All properties of the nuclear system in the chosen model space, and with the chosen interaction, are then defined, and one expects to get better and better results (as compared with experiment) by enlarging the model space and improving the model interaction. But, in practice, this soon becomes impossible since, even for relatively small values of m and N (and even if there are simplifying symmetries), the dimensionalities of the matrices to be constructed and diagonalized become too large to handle even for the most sophisticated computers.

The purpose of statistical nuclear spectroscopy is to overcome this limitation by essentially starting at the other end of the problem. The idea is to look at the global properties of the Hamiltonian and other operators in the model space, and at the correlations between them. Some general properties of the system can be obtained most readily this way.[6] Level densities and spectra can also be constructed from the moments.[6,7]. In fact, at least in finite-dimensional model spaces, one could in principle produce all the microscopic details by evaluating moments and covariances up to the order determined by the dimensionality of the model space. But this, by itself, would not be of much practical significance, if it were not for the existence of two helpful factors that contribute towards making this approach more successful than would be presumed otherwise.

The first simplifying factor derives from the recognition of the role played by a central limit theorem[6] (CLT) in many-particle model spaces constructed by distributing nucleons over some finite set of single-particle states. Then, by virtue of this CLT, in the limit of large particle number, the smoothed eigenvalue distributions for most Hamiltonian operators in the model space become[6,8] close to Gaussian. This, in turn, implies[9] closely related characteristic asymptotic forms, for expectation values and strengths of other operators, defined by only a small number of traces over the model space of operators and their products. Such operator traces can be calcuated[10,11] by methods which do not involve construction of any Hamiltonian eigenfunctions. The fact that such traces can be obtained[6] in a many-particle space by "propagation" from lower particle spaces is the second simplifying factor. This requires one to evaluate those traces only in a minimum defining set of spaces of low particle or hole number. These two features make the statistical approach attractive, especially in model spaces of large dimensionality. Moreover, by its very nature, it gives results as more or less explicit functions of the Hamiltonian matrix elements so that one can easily connect the features of the Hamiltonian with the corresponding properties of the strengths and expectation values.

The purpose here is to extend this statistical approach to inverse-energy-weighted sum-rules so that we can evaluate them in terms of traces of operators and operator products without having to know their eigenvalues and eigenfunctions. For this, we first reformulate the conventional Rayleigh–Schrödinger perturbation theory[12] in terms of parametric derivatives of a distribution function and then derive an orthogonal polynomial expansion for the same. We also derive the result in the CLT limit and indicate some applications. Before we do all this, let us familiarize our-

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 0022-2488/81/122961-07$01.00

selves with a special set of orthonormal polynomials that are used in statistical nuclear theory. As usual we take the system to consist of m nucleons in N single-particle states with two-body interactions between the nucleons. But some of the results derived in this paper (those in Sec. 4A) seem to be applicable more generally. Moreover, all the results apply for both discrete and continuous spectral densities $\rho(W)$.

2. ORTHONORMAL POLYNOMIALS

Let H be the Hamiltonian for the nuclear system and $\rho(W)$ denote the density of states at energy W. Let d be the dimensionality of the model space. Associated with the density $\rho(x)$is a complete set of orthonormal polynomials P_μ such that

$$\int P_\mu(x)P_\nu(x)\rho(x)\,dx = \delta_{\mu\nu}, \tag{1}$$

$$\delta(x-y) = \rho(x)\sum_\mu P_\mu(x)P_\mu(y). \tag{2}$$

These polynomials can be constructed explicitly in terms of the density moments

$$M_p = \int \rho(z)z^p\,dz = \langle H^p\rangle^m = \frac{1}{d}\langle\langle H^p\rangle\rangle^m, \tag{3}$$

where we use the notation that, for any operator G, $\langle\langle G\rangle\rangle^m$ denotes the trace over the model space and $\langle G\rangle^m$ denotes the average expectation value. The first two polynomials are

$$P_0(z) = 1, \quad P_1(z) = (z-\mathscr{E})/\sigma, \tag{4}$$

where $\mathscr{E} = M_1$ and $\sigma^2 = M_2 - M_1^2$ are the centroid and variance. The polynomial of order ν requires density moments of orders up to 2ν and is given by[13]

$$[D_{\nu-1}D_\nu]^{1/2}P_\nu(z) = \begin{vmatrix} 1 & M_1 & M_2 \ldots & M_\nu \\ M_1 & M_2 & \ldots & M_{\nu+1} \\ M_{\nu-1} & M_\nu & \ldots & M_{2\nu-1} \\ 1 & z & z^2 \ldots & z^\nu \end{vmatrix}, \tag{5}$$

where D_ν is the determinant in Eq. (5) with the last row replaced by $[M_\nu, M_{\nu+1}, \ldots, M_{2\nu}]$.

When the density is Gaussian, i.e.,

$$\rho(W) = (2\pi\sigma^2)^{-1/2}\exp\{-(W-\mathscr{E})^2/2\sigma^2\}, \tag{6}$$

the polynomials P_μ are related to the Hermite polynomials H_μ by

$$P_\mu(W) = (\mu!)^{-1/2}He_\mu\{(W-\mathscr{E})/\sigma\}, \tag{7}$$

where

$$He_\mu(z) = 2^{-\mu/2}H_\mu(z/\sqrt{2}).$$

When the density is of chi-squared type, the P_μ are related to the Laguerre polynomials.

In terms of the orthogonal polynomials $P_\mu(x)$ one derives[9] for the expectation value of an operator K,

$$\begin{aligned} K(W) &\equiv \langle W|K|W\rangle \\ &= (d\rho(W))^{-1}\langle\langle K\delta(H-W)\rangle\rangle^m \\ &= \sum_\mu \langle KP_\mu(H)\rangle^m P_\mu(W). \end{aligned} \tag{8}$$

This polynomial expansion is found[9] to be rapidly convergent due to the action of a central limit theorem in many particle model spaces. This will be discussed in more detail later. $K(W)$ in Eq. (8) involves only traces of products of operators. These traces can be evaluated without having to know eigenvalues and eigenfunctions. In addition, because of the rapid convergence, we need only traces of low order and they can be evaluated[10,11] fairly easily even for systems of large dimensionality.

We seek to obtain such a formalism for the inverse-energy-weighted sum-rules (IEWSR). First we review, very briefly, convergence and the central limit theorem.

3. CENTRAL LIMIT THEOREM AND CONVERGENCE

As noted earlier the many particle nature of the model space ensures rapid convergence of the polynomial expansion (8). It has been known for many years now that as we increase the number of particles, the model space eigenvalue density goes rapidly to Gaussian, as a consequence of the central limit theorem. In the case of noninteracting particles this comes about because the density convolutes as we add particles. Thus,

$$\begin{aligned} \rho_m(x) &= \int \rho_{m-1}(x-y)\rho_1(y)\,dy \equiv \rho_{m-1}\otimes\rho_1[x] \\ &= \rho_1\otimes\rho_1\otimes\rho_1\otimes\ldots\otimes\rho_1[x], \end{aligned} \tag{9}$$

in which m stands for the particle number. The density of energy states for the m-particle system is then an m-fold convolution of the single-particle energy density. Then, by the simplest version of CLT, $\rho_m(x)$ approaches Gaussian for large enough particle number (for characteristic single-particle spectra $m \gtrsim 6$ is enough for a good Gaussian).

The convolution argument given above requires that the energies of the different particles be additive and independent. These conditions are not met for a system of interacting nucleons. The Pauli blocking effect (which can be ignored for dilute systems, i.e., $m \ll N$) violates statistical independence, and additivity is violated if interactions have to be considered. Despite all this it is found[8] that all nuclear Hamiltonians which give reasonable agreement with experimental data have model space spectra which are close to Gaussian. This is better understood[1] by studying an ensemble of Hamiltonians of two-body interactions. It is found that the ensemble-averaged density is Gaussian, and that for large systems ($1 \ll m \ll N$) only a negligible fraction of the members of the ensemble give deviant densities. However, in actual calculations, corrections to Gaussian are often necessary and can be easily incorporated.

The convergence of the density to Gaussian implies an asymptotic linearity in $K(W)$, which is then given by the first two terms of Eq. (8).

$$K(W) \overset{\text{CLT}}{\to} \langle K\rangle + \langle K(H-\langle H\rangle)\rangle(W-\langle H\rangle)/\sigma^2. \tag{10}$$

This can be interpreted by a linear geometry in the model space of operators. It could also have been derived[14] by a linear response theory. In fact we shall use the response theory approach in the following to treat inverse-energy-weighted sum rules.

4. PERTURBATION THEORY

A. Distribution function approach

Consider a perturbation of the Hamiltonian H by αK where α is a small parameter and K is the perturbing operator. Let E and E_α denote the corresponding eigenvalues of H and $H_\alpha \equiv H + \alpha K$, respectively. Let E_α be expressed as a power series in α by

$$E_\alpha = E + \alpha S_1(E) + \alpha^2 S_2(E) + \cdots$$

$$= \sum_{n=0}^{\infty} \alpha^n S_n(E) \quad \text{where } S_0(E) = E. \tag{11}$$

This definition implies that the $S_n(E)$ are the same as the terms in the Rayleigh–Schrödinger perturbation series. In particular,

$$S_1(E) = \langle E|K|E\rangle, \tag{12}$$

$$S_2(E) = -\sum_{E' \neq E} \frac{|\langle E'|K|E\rangle|^2}{E' - E}. \tag{13}$$

Denote the density (normalized to unity) of eigenvalues of H and H_α by ρ and ρ_α, respectively and the corresponding pth moments by M_p and $M_p(\alpha)$. Now $M_p(\alpha)$ can be written in two different ways. By the standard definition of moment,

$$M_p(\alpha) = \int_{-\infty}^{\infty} x^p \rho_\alpha(x)\, dx. \tag{14}$$

However, the perturbation $H \to H_\alpha$ takes the eigenvalue E to E_α. The number of eigenvalues E which thus go to E_α is $\rho(E)\, dE$. Then

$$M_p(\alpha) = \int_{-\infty}^{\infty} (E_\alpha)^p \rho(E)\, dE. \tag{15}$$

The reader should be able to visualize this important relation by taking the example of a discrete spectrum. Denoting $D^n \equiv \partial^n/\partial\alpha^n$ for all $n > 0$, we have, by repeated application of the Liebnitz theorem in differential calculus,

$$D^n((E_\alpha)^p) = \prod_{r=1}^{p} \left[\sum_{i_r=0}^{n-\sum_{k=0}^{r-1} i_k} \binom{n - \sum_{k=0}^{r-1} i_k}{i_r} (D^{i_r} E_\alpha) \right], \tag{16}$$

where $i_0, i_1, i_2, \ldots, i_p$ are such that

$$i_0 = 0, \quad i_1 + i_2 + \cdots + i_p = n, \quad \text{and each } i_r \geqslant 0.$$

But, from Eq. (11),

$$D^l E_\alpha = \sum_{n=l}^{\infty} \binom{n}{l} l!\, \alpha^{n-l} S_n. \tag{17}$$

Then it follows from Eq. (15) that

$$D^n M_p(\alpha)\big|_{\alpha=0}$$

$$= \int_{-\infty}^{\infty} \rho(E) \left[\prod_{r=1}^{p} \sum_{i_r=0}^{n-\sum_{k=0}^{r-1} i_k} \binom{n - \sum_{k=0}^{r-1} i_k}{i_r} i_r! S_{i_r}(E) \right] dE \tag{18}$$

$$= \int_{-\infty}^{\infty} \rho(E) \sum_{t=1}^{n} E^{p-t} a_t^n(E)\, dE, \tag{19}$$

where the coefficient $a_t^n(E)$ is given below by Eq. (21). Equation (19) is obtained from (18) by the following argument: When any of the indices $i_1, i_2, \ldots, i_p$ in Eq. (18) is zero, it contributes a factor $S_0(E) = E$ to the corresponding term. Then we collect together all the terms having a fixed number t (where $t = 1,2,\ldots,n$) of these indices as nonzero and the rest $(p - t)$ zero. For each choice of the set of nonzero values, the $(p - t)$ zeroes can be chosen in $\binom{p}{t}$ ways and each of those ways would contribute the same term to Eq. (18). Then we can fix the indices i_r such that $i_1, i_2, \ldots, i_t$ are nonzero and $i_{t+1}, \ldots, i_p$ are zero. Therefore,

$$i_1 + i_2 + \cdots + i_t = n \tag{20}$$

and the coefficient $a_t^n(E)$ has the E-dependent factors $\binom{p}{t} S_{i_1}(E) S_{i_2}(E) \cdots S_{i_t}(E)$ which should further be multiplied by the number of ways in which $i_1, \ldots, i_p$ can be chosen such that $i_1, i_2, \ldots, i_t$ are nonzero (and positive integers) and satisfy the condition $i_1 + i_2 + \cdots + i_t = n$ (the rest being zero). This number is equivalent to the number of ways in which n identical things can be put into t boxes with at least one in each of them, or the number of partitions of the number n into t positive terms. Denoting such partitions by P [there are $\binom{n-1}{t-1}$ of them], we can write for $a_t^n(E)$ the expression

$$a_t^n(E) = \binom{p}{t} \sum_P \binom{n}{i_1} \binom{n - i_1}{i_2} \cdots \binom{n - \sum_{k=0}^{t-1} i_k}{i_t}$$

$$\times i_1! i_2! \cdots i_t! S_{i_1}(E) S_{i_2}(E) \cdots S_{i_t}(E). \tag{21}$$

Now integrate the right-hand side of Eq. (19) by parts t times to get

$$\left.\frac{\partial^n M_p(\alpha)}{\partial \alpha^n}\right|_{\alpha=0} = \sum_{t=1}^{n} \int_{-\infty}^{\infty} E^p \frac{\partial^t}{\partial E^t} [\rho(E) c_t^n(E)]\, dE, \tag{22}$$

where

$$c_t^n(E) = (-1)^t \binom{p}{t}^{-1} (t!)^{-1} a_t^n(E)$$

$$= (-1)^t \frac{n!}{t!} \sum_P S_{i_1}(E) S_{i_2}(E) \cdots S_{i_t}(E), \tag{23}$$

where the partitions P are such that

$$\sum_{k=1}^{t} i_k = n, \quad i_k \geqslant 1.$$

Equation (22) can now be written as

$$\int_{-\infty}^{\infty} \left[\left.\frac{\partial^n \rho_\alpha}{\partial \alpha^n}\right|_{\alpha=0} - \sum_{t=1}^{n} \frac{\partial^t}{\partial E^t} (\rho(E) c_t^n(E)) \right] E^p\, dE = 0, \tag{24}$$

for all p. The term within square brackets in the above equation then vanishes, and on integrating it with respect to E, we get

$$\left.\frac{\partial^n F_\alpha(E)}{\partial \alpha^n}\right|_{\alpha=0} = \sum_{t=1}^{n} \frac{\partial^{t-1}}{\partial E^{t-1}} (\rho(E) c_t^n(E)). \tag{25}$$

Here $F_\alpha(E)$ is the distribution function $\int_{-\infty}^{E} \rho_\alpha(x)\, dx$. Since

$$c_1^n(E) = -n! S_n(E), \tag{26}$$

we can write

$$S_n(E) = -\frac{1}{n!} \frac{1}{\rho(E)}$$

$$\times \left[\left.\frac{\partial^n F_\alpha(E)}{\partial \alpha^n}\right|_{\alpha=0} - \sum_{t=1}^{n-1} \frac{\partial^t}{\partial E^t} (\rho(E) c_{t+1}^n(E)) \right], \tag{27}$$

where $c_l^n(E)$ is given by Eq. (23). Equation (27) expresses $S_n(E)$, the nth order term in the perturbation series (11), in terms of the nth parametric derivative of $F_\alpha(E)$ and the lower order terms $S_l(E)$ for $l<n$, which themselves are given in terms of lower order parametric derivatives of $F_\alpha(E)$. Thus we are able to relate $S_n(E)$ to the parametric derivatives of $F_\alpha(E)$ up to the nth order.

When $n=1$, Eq. (27) gives the already known[14] result for the expectation value of K, viz.,

$$K(E)\equiv S_1(E)=-\frac{1}{\rho(E)}\frac{\partial F_\alpha(E)}{\partial\alpha}\bigg|_{\alpha=0}. \tag{28}$$

When $n=2$ we get the expression for the second-order perturbation term or the first inverse-energy-weighted sum,

$$S_2(E)=-\frac{1}{2\rho(E)}\times\left[\frac{\partial^2F_\alpha}{\partial\alpha^2}\bigg|_{\alpha=0}-\frac{\partial}{\partial E}\left[\frac{1}{\rho(E)}\left(\frac{\partial F_\alpha}{\partial\alpha}\bigg|_{\alpha=0}\right)^2\right]\right], \tag{29}$$

and the explicit form for $n=3$ is

$$S_3(E)=-\frac{1}{6\rho(E)}\left[\frac{\partial^3F_\alpha}{\partial\alpha^3}\bigg|_{\alpha=0}-6\frac{\partial}{\partial E}[\rho(E)S_1(E)S_2(E)+\frac{\partial^2}{\partial E^2}(\rho(E)(S_1(E))^3)\right]. \tag{30}$$

B. CLT result

Characterizing the distribution $\rho(x)$ by its centroid $s_1\equiv\xi$, variance $s_2\equiv\sigma^2$ and a set of translation and scale invariant shape parameters s_ν, $\nu\geqslant3$, we can write

$$\frac{\partial F_\alpha}{\partial\alpha}=\sum_\nu\frac{\partial s_\nu}{\partial\alpha}\frac{\partial F_\alpha}{\partial s_\nu} \tag{31}$$

and

$$\frac{\partial^2F_\alpha}{\partial\alpha^2}=\sum_\nu\frac{\partial^2s_\nu}{\partial\alpha^2}\frac{\partial F_\alpha}{\partial s_\nu}+\sum_\nu\frac{\partial s_\nu}{\partial\alpha}\sum_\mu\frac{\partial s_\mu}{\partial\alpha}\frac{\partial^2F_\alpha}{\partial s_\mu\partial s_\nu}. \tag{32}$$

In the CLT limit, we assume $\rho_\alpha(x)$ to be Gaussian with centroid ξ_α and width σ_α {more generally, we can take $\rho_\alpha(x)$ to be of the form $(1/\sigma_\alpha)f[(x-\xi_\alpha)/\sigma_\alpha]$}, and then the $\nu\geqslant3$ terms in Eqs. (31) and (32) do not contribute. Moreover,

$$\frac{\partial F_\alpha(E)}{\partial s_1}=-\rho_\alpha(E), \tag{33}$$

$$\frac{\partial F_\alpha(E)}{\partial s_2}=-\left\{\frac{E-\xi_\alpha}{2\sigma_\alpha^2}\rho_\alpha(E)\right\}, \tag{34}$$

$$\frac{\partial^2F_\alpha(E)}{\partial s_1^2}=\frac{\partial\rho_\alpha(E)}{\partial E}, \tag{35}$$

$$\frac{\partial^2F_\alpha(E)}{\partial s_2^2}=\frac{(E-\xi_\alpha)}{4\sigma_\alpha^4}\left\{(E-\xi_\alpha)\frac{\partial\rho_\alpha(E)}{\partial E}+3\rho_\alpha(E)\right\}, \tag{36}$$

$$\frac{\partial^2F_\alpha(E)}{\partial s_2\partial s_1}=\frac{\partial^2F_\alpha(E)}{\partial s_1\partial s_2}=\frac{E-\xi_\alpha}{2\sigma_\alpha^2}\frac{\partial\rho_\alpha(E)}{\partial E}+\frac{\rho_\alpha(E)}{2\sigma_\alpha^2}. \tag{37}$$

In addition,

$$\frac{\partial s_1}{\partial\alpha}\bigg|_{\alpha=0}=\langle K\rangle^m, \tag{38}$$

$$\frac{\partial^2s_1}{\partial\alpha^2}\bigg|_{\alpha=0}=0, \tag{39}$$

$$\frac{\partial s_2}{\partial\alpha}\bigg|_{\alpha=0}=2\zeta\sigma_K\sigma, \tag{40}$$

$$\frac{\partial^2s_2}{\partial\alpha^2}\bigg|_{\alpha=0}=2\sigma_K^2, \tag{41}$$

where $\zeta=\langle(H-\xi)(K-\langle K\rangle)\rangle/\sigma_K\sigma$ is the correlation coefficient between H and K, σ_K^2 is the variance of K. Then using Eq. (31) to (41) in Eq. (29), for $S_2(E)$ we get

$$S_2(E)=(1-\zeta^2)(\sigma_K^2/2\sigma^2)(E-\xi). \tag{42}$$

This is the desired CLT result for IEWSR.

C. Polynomial expansions

We now obtain an expansion for the perturbation term $S_2(E)$ in terms of orthogonal polynomials defined by the moments of the density. The $\nu=1$ and $\nu=2$ contributions to $\partial F_\alpha/\partial\alpha$ and $\partial^2F_\alpha/\partial\alpha^2$ in Eqs. (31) and (32) have been obtained above and now we evaluate the $\nu\geqslant3$ terms. For this, we choose[9] the shape parameters $s_{\nu\geqslant3}(\alpha)$ to be the νth order polynomial moments of the form

$$s_\nu(\alpha)=\int\rho_\alpha(z)V_\nu(z)\,dz,\quad\text{for }\nu\geqslant3 \tag{43}$$

$$=\langle V_\nu(H+\alpha K)\rangle, \tag{44}$$

where $V_\nu(z)$ is a νth order polynomial in which the coefficient of z^ν does not vanish. The precise form of $V_{\nu\geqslant3}(z)$ will be chosen later. However, they must be functions of $(z-\xi)/\sigma$ only, so that the invariance requirements of the shape parameters are satisfied. The deformed density and distribution functions are

$$\rho_\alpha(z)=g_\alpha(z)\left\{1+\sum_{\nu\geqslant3}s_\nu(\alpha)T_\nu(z)\right\}, \tag{45}$$

$$F_\alpha(z)=\int_{-\infty}^{z}\rho_\alpha(x)\,dx. \tag{46}$$

Here the centroid and variance deformations are included in $g_\alpha(z)$, which is a function of the form $(1/\sigma)f[(z-\xi)/\sigma]$, and $T_\nu(z)$ is another set of polynomial functions of $(z-\xi)/\sigma$. It follows from Eqs. (43) and (45) that the two sets of polynomials $V_\nu(z)$ and $T_\nu(z)$ are related by an orthonormality condition

$$\int g(z)V_\nu(z)T_\mu(z)\,dz=\delta_{\mu\nu}\quad\text{for }\nu\geqslant3,\ \mu\geqslant3. \tag{47}$$

Thus we can make[9] the following choice for $V_\nu(z)$ and $T_\nu(z)$

$$V_\nu'(z)=P_{\nu-1}(z), \tag{48}$$

$$g(z)T_\nu(z)=-\frac{d}{dz}(\rho(z)P_{\nu-1}(z)), \tag{49}$$

where $P_\nu(z)$ are orthonormal polynomials associated with the density $\rho(z)$. Then,

$$\frac{\partial s_\nu}{\partial\alpha}\bigg|_{\alpha=0}=\langle KP_{\nu-1}(H)\rangle, \tag{50}$$

$$\frac{\partial^2s_\nu}{\partial\alpha^2}\bigg|_{\alpha=0}=\left\langle\frac{\partial^2}{\partial\alpha^2}V_\nu(H+\alpha K)\bigg|_{\alpha=0}\right\rangle. \tag{51}$$

Further, it is straightforward to show that (with $\mu\geqslant\nu$, $\nu\geqslant3$),

$$\frac{\partial F(E)}{\partial s_\nu} = -\rho(E)P_{\nu-1}(E), \tag{52}$$

$$\frac{\partial^2 F(E)}{\partial s_1 \partial s_\nu} = \frac{\partial}{\partial E}\{\rho(E)P_{\nu-1}(E)\}, \tag{53}$$

$$\frac{\partial^2 F(E)}{\partial s_2 \partial s_\nu} = \frac{E-\xi}{2\sigma^2}\frac{\partial}{\partial E}\{\rho(E)P_{\nu-1}(E)\}, \tag{54}$$

$$\frac{\partial^2 F(E)}{\partial s_\mu \partial s_\nu} = 0. \tag{55}$$

Now, using Eqs. (50)–(55) in Eqs. (31) and (32), we get, from Eq. (29),

$$\begin{aligned} S_2(E) = (1-\zeta^2)\frac{\sigma_K^2}{2\sigma^2}(E-\xi) \\ + \frac{1}{2}\sum_{\mu\geq 2}\left(\frac{\partial^2 s_{\mu+1}}{\partial\alpha^2}\right)_{\alpha=0} P_\mu(E) \\ + \sum_{\mu\geq 2}\langle KP_\mu(H)\rangle\langle KP_1(H)\rangle\frac{1}{\sigma}P_\mu(E) \\ + \sum_{\mu\geq 2}\sum_{\nu\geq 2}\langle KP_\mu(H)\rangle\langle KP_\nu(H)\rangle \\ \times\rho^{-1}(E)\frac{d}{dE}\{\rho(E)P_\mu(E)P_\nu(E)\}, \end{aligned} \tag{56}$$

where $(\partial^2 s_\mu/\partial\alpha^2)_{\alpha=0}$ has the form

$$\sum_{r=0}^{\mu} r\beta_r^\mu \sum_{l=0}^{r-2}\langle KH^l KH^{r-l-2}\rangle, \tag{57}$$

where the coefficients β_r^μ are such that

$$V_\mu(z) = \sum_r \beta_r^\mu z^r. \tag{58}$$

5. EXAMPLE AND APPLICATIONS

A. A two-level example

We shall first look at a two-level system and demonstrate the equivalence of the Rayleigh–Schrödinger theory and the distribution function formalism of perturbation theory as developed here. It is also instructive to apply the CLT result to the two-level case.

Let a and b be the two eigenvalues ($a<b$) of a two-level system with Hamiltonian H. Then

$$\rho(E) = \tfrac{1}{2}[\delta(E-a)+\delta(E-b)]. \tag{59}$$

Suppose

$$K = \begin{pmatrix} u & g^* \\ g & v \end{pmatrix} \tag{60}$$

is a perturbation on H and $H\to H_\alpha \equiv H+\alpha K$. The second-order corrections to the eigenvalues of H_α, by the Rayleigh–Schrödinger theory, are given by

$$S_2(a) = gg^*/(a-b), \quad S_2(b) = gg^*/(b-a). \tag{61}$$

The eigenvalues a_α and b_α of H_α are easily calculated as the solutions of the characteristic equation $|H_\alpha - \lambda I| = 0$ where I is the unit matrix. This equation is

$$\lambda^2 - \lambda(a+b+\alpha(u+v)) + (a+\alpha u)(b+\alpha v) - \alpha^2 gg^* = 0. \tag{62}$$

In terms of the roots a_α and b_α of Eq. (62) we have

$$F_\alpha(E) = \frac{1}{2}\int_{-\infty}^{E}[\delta(x-a_\alpha)+\delta(x-b_\alpha)]\,dx. \tag{63}$$

Note that for a_α and b_α,

$$\left.\frac{\partial a_\alpha}{\partial\alpha}\right|_{\alpha=0} = u, \quad \left.\frac{\partial b_\alpha}{\partial\alpha}\right|_{\alpha=0} = v, \tag{64}$$

$$\left.\frac{\partial^2 a_\alpha}{\partial\alpha^2}\right|_{\alpha=0} = \frac{2gg^*}{a-b}, \quad \left.\frac{\partial^2 b_\alpha}{\partial\alpha^2}\right|_{\alpha=0} = -\frac{2gg^*}{a-b}. \tag{65}$$

We then have

$$\left.\frac{\partial F_\alpha}{\partial\alpha}\right|_{\alpha=0} = \frac{1}{2}[u\delta(E-a)+v\delta(E-b)], \tag{66}$$

$$\begin{aligned} \left.\frac{\partial^2 F_\alpha}{\partial\alpha^2}\right|_{\alpha=0} = \frac{gg^*}{a-b}\delta(E-a) + \frac{gg^*}{b-a}\delta(E-b) \\ + \tfrac{1}{2}u^2\delta'(E-a) + \tfrac{1}{2}v^2\delta'(E-b). \end{aligned} \tag{67}$$

Equation (29) can now be used to get

$$S_2(E)\rho(E) = \tfrac{1}{2}\left[\frac{gg^*}{a-b}\delta(E-a) + \frac{gg^*}{b-a}\delta(E-b)\right], \tag{68}$$

which is exactly what the Rayleigh–Schrödinger theory suggested.

We also consider the CLT result for this two-level system. Now

$$\mathscr{E} = \tfrac{1}{2}(a+b), \tag{69}$$

$$\sigma^2 = [\tfrac{1}{2}(a-b)]^2, \tag{70}$$

$$\sigma_K^2 = \tfrac{1}{4}[(u-v)^2 + 4gg^*], \tag{71}$$

$$\zeta^2 = (u-v)^2/[(u-v)^2 + 4gg^*]. \tag{72}$$

Then, by Eq. (42), the CLT would predict

$$S_2(E) = [2gg^*/(a-b)^2][E - \tfrac{1}{2}(a+b)] \tag{73}$$

for the two-level system. This is the straight line passing through the exact values $S_2(a)$ and $S_2(b)$ in Eq. (61). The CLT result is thus a smoothed linear approximation of the exact behavior as one might have expected in this case.

B. Perturbation theory

One obvious application is to calculate the effect of a perturbation on the known eigenvalues of an otherwise unperturbed operator.

As an illustration we take the particular case of the recently developed statistical approximation[15] to model interactions in nuclear physics. In that development, which we review briefly, an algorithm was proposed for expanding any interaction in terms of a given set of operators, one motivation for doing so being the study of the types of forces that dominate an interaction. The theoretical basis for the construction is a model space geometry which emphasizes the importance of traces of bilinear products of operators and is made effective by the operation of the central limit theorem.

For any operator O defined in the model space,

$$\langle O^+ O\rangle^m = ||O||_m^2 \tag{74}$$

is the square of a proper norm. Furthermore,

$$\langle O_\alpha{}^+ O_\beta\rangle^m/||O_\alpha||_m||O_\beta||_m = \cos\theta_{\alpha\beta} \tag{75}$$

defines an inner product. We have a linear vector space here and we can make use of the results of linear algebra. So if $(O_1,O_2,...,O_k)$ is a set of independent operators defined in our space, then

$$H = c_1O_1 + c_2O_2 + \cdots + c_kO_k + X. \tag{76}$$

If $\{O_\alpha\}$ is complete, then X vanishes. The c_α can be determined from the $\langle O_\alpha{}^+H\rangle^m$ and $\langle O_\alpha{}^+O_\beta\rangle^m$ by matrix inversion. The norm of $(H-X)$ compared to the norm of H provides a measure for the completeness of the expansion.

By a proper choice of the operators O_α, one can use this technique to study group symmetries and to gain physical insight into the types of forces that dominate an interaction.

In one such example, the Brown–Kuo Hamiltonian[16] H was approximated by an extended French trace-equivalent (FTE) operator[15] H'(FTE), which looked after the orbital and isospin structure of H and also included projections of H along P (pairing operator), G_2 [second-order U(4) Casimir invariant], $Q\cdot Q, L^2, S^2$, and J^2. This H'(FTE) accounted for about 97% of the full width of H. Then

$$H = H'(\text{FTE}) + H^R, \tag{77}$$

where H^R is the residual part of H.

We now treat H^R as a pertubation on H'(FTE) and calculate the ground-state energy E_0 of H from the ground-state energy E_0' of H'(FTE). Then, using the CLT result and the fact that H' and H^R are orthogonal, we get (up to second-order in perturbation theory)

$$E_0 \simeq E_0' + \tfrac{1}{2}(E_0' - \langle H'\rangle)\left[\frac{\sigma_H^2}{\sigma_{H'}^2} - 1\right]. \tag{78}$$

In $(ds)^6$, E_0' has the value -59.46 MeV (where H is the Brown–Kuo Hamiltonian), the perturbation correction turns out to be -0.95 MeV, giving a value -60.41 MeV for E_0. The exact value of E_0, obtained by shell-model is -60.35 MeV.

C. Moment of inertia

Using the cranking model,[17] the moment of inertia of a nucleus can be expressed as an IEWSR. It is obtained by evaluating the energy increase when the intrinsic (body-fixed) wavefunction is rotated. Suppose the intrinsic wavefunction or body-fixed frame is rotating about the x axis with angular velocity ω. The wavefunction for the rotating nucleus expressed in space-fixed coordinates is a solution of the time-dependent Schrödinger equation

$$H\phi_\omega(r,t) = i\hbar\frac{\partial}{\partial t}\phi_\omega(r,t). \tag{79}$$

But $\phi_\omega(r,t)$ must be stationary in the body-fixed frame. Then

$$\hat{\phi}_\omega(r,t) = e^{i\omega tJ_x}\phi_\omega(r,t) \tag{80}$$

is stationary in the space-fixed frame. Now, inserting (80) into (79),

$$H\hat{\phi}_\omega(r,t) = i\hbar\frac{\partial}{\partial t}\hat{\phi}_\omega(r,t) + \hbar\omega J_x\hat{\phi}_\omega(r,t). \tag{81}$$

For $\hat{\phi}_\omega(r,t)$ to be stationary, it must have the form

$$\hat{\phi}_\omega(r,t) = \hat{\phi}_\omega(r)e^{-iE(\omega)t/\hbar}. \tag{82}$$

and $\hat{\phi}_\omega(r)$ must obey the equation

$$(H - \hbar\omega J_x)\hat{\phi}_\omega(r) = E(\omega)\hat{\phi}_\omega(r). \tag{83}$$

Then, using Rayleigh–Schrödinger perturbation theory

$$E(\omega) = E_0 + \omega^2\hbar^2\sum_{i\neq 0}\frac{|\langle i|J_x|0\rangle|^2}{E_i - E_0}, \tag{84}$$

so that the moment of inertia is

$$\mathscr{I}_x = 2\hbar^2\sum_{i\neq 0}\frac{|\langle i|J_x|0\rangle|^2}{E_i - E_0}. \tag{85}$$

To evaluate $\mathscr{I}_x$ one normally feeds in the wavefunctions and energies from a model for the intrinsic structure. It can be evaluated analytically in special cases like a pure deformed harmonic oscillator potential without spin-orbit or residual interactions. A proper model should include these features also in the Hamiltonian. But then evaluation by conventional methods becomes difficult.

Using the CLT result (42) for IEWSR derived in this paper, we can write

$$\mathscr{I}_x = 2\hbar^2(1 - \zeta^2_{J_x,H})\frac{\sigma^2_{J_x}}{2\sigma^2_H}(E_0 - \langle H\rangle), \tag{86}$$

where E_0 is the ground-state energy. We make here a simple calculation using a Nilsson one-body Hamiltonian[18] which consists of an anisotropic harmonic oscillator well, together with a single-particle spin-orbit force and a quadratic orbital angular momentum force

$$H = \sum_i\Big[-\frac{\hbar^2}{2M}\nabla_i^2 + \tfrac{1}{2}M\omega_0^2(\epsilon)\{(x_i^2 + y_i^2)(1 + \tfrac{1}{3}\epsilon)^2 + z_i^2(1 - \tfrac{2}{3}\epsilon)^2\} + Cl_i\cdot s_i + Dl_i^2\Big], \tag{87}$$

where ϵ is the deformation parameter, C and D are chosen to reproduce the known shell-model level sequence at zero deformation. Using the single-particle energy levels for this Nilsson Hamiltonian as tabulated in Ref. 18, we evaluated the CLT result for moment of inertia. A value of 59 $\hbar^2$ was obtained for the nucleus ^{166}Ho. The experimental value is 55 $\hbar^2$ and the rigid body value is 70 $\hbar^2$. A thorough study of moment of inertia of deformed nuclei taking into account pairing and other two-body correlations will be made in the future.

D. Other applications

Perturbation and IEWSR are used in several other places in nuclear physics, like the vibrating potential model,[17] effective charges,[19] effective interaction theory[20] and so on. Applications in other branches of physics also need to be looked into.

6. SUMMARY

A statistical approach to the many nucleon problem has been extended here to the treatment of perturbations and inverse-energy-weighted sum-rules. The first IEWSR, denoted by S_2, for an excitation operator K is defined by Eq. (13). Because of the energy denominator, this quantity is largely determined by the low-lying excitations and hence is

of interest in the study of collectivity, moment of inertia, etc. It also represents the second-order term in the Rayleigh–Schrödinger series for the perturbation $H \to H + \alpha K$. We have developed a statistical perturbation theory, and then derived a polynomial expansion for $S_2(E)$. The most important new results derived here are Eq. (29) for $S_2(E)$ and the general result (27) for $S_n(E)$. In the CLT convergence limit, one gets the linear result (42) for $S_2(E)$. Corrections to this from the shape parameters of the density are given in the form of a polynomial expansion, Eq. (56). Further, we presented a test application to calculate the perturbed eigenvalue and a simple application to the moment of inertia in nuclei. The results were very encouraging.

ACKNOWLEDGMENTS

The author is grateful to Professor J. B. French for discussions, guidance, and support. Helpful discussions with Dr. B. D. Chang, Professor D. S. Koltun, and Professor P. C. Sood are also acknowledged. Further thanks are due to Professor L. Zamick and Professor A. Mekjian for their hospitality and support at Rutgers.

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A calculation of the Casimir force on a circular boundary

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(Received 28 August 1980; accepted for publication 24 October 1980)

The zero point energy of a three-dimensional scalar field in the presence of a circular boundary of radius R is calculated using a Green's function method. It is found that the energy is cutoff-dependent. The cutoff-dependent terms are explicitly calculated in terms of the geometry of the problem. It is found that

$$E(\omega_0) = +\frac{0.045}{2R} + \frac{S}{4\pi}\omega_0^2 - \left[\frac{1}{256}\int c^2(s)\,ds\right]\ln\omega_0 R,$$

where S is the length of circular boundary ($S = 2\pi R$), $c(s)$ the curvature of the boundary [$c(s) = 1/R$], and ω_0 is the cutoff frequency.

PACS numbers: 41.10.Fs

I. INTRODUCTION

Recently there has been some interest in the Casimir effect.[1] The original "Casimir effect"[2] was an observable nonclassical force of attraction between two perfectly conducting plates. Casimir was led to predicting such a force by considering the zero point energy of a scalar field between the two plates.

In this paper we will calculate the zero point energy of a three-dimensional scalar field (2-space + 1-time) in the presence of a circular boundary. We will call this energy the Casimir energy of the system. Our calculational procedure is based on a Green's function method similar to that of Bender and Hays[3] and of Milton, DeRaad, and Schwinger.[4] The motivation for the calculation was to see what happens to the Casimir energy when we change the dimensionality of space. In three spatial dimensions the Casimir force is attractive between parallel plates[2] but repulsive for a sphere.[4–7] What are the corresponding results in two spatial dimensions? In Sec. II the Green's function method which we will use to do our calculation is briefly explained. In Sec. III the method is applied to the case of a circular boundary. In Sec. IV the general expression for the Casimir energy is evaluated using the uniform asymptotic expansion technique employed by Milton, DeRaad, and Schwinger.[4] Numerical evaluation of various integrals is also carried out. The finite part of the Casimir energy is found to be

$$E_{\text{finite}} = +0.045/(2R). \tag{1.1}$$

In Sec. V the divergent or cutoff-dependent parts of the Casimir energy are discussed. The expression for the Casimir energy $E(\omega_0)$, including the cutoff-dependent term is

$$E(\omega_0) = 0.045/(2R) - (1/R)\cdot\tfrac{1}{128}\ln\omega_0 R + \tfrac{1}{2}R\omega_0^2. \tag{1.2}$$

It is shown in Sec. V, by explicit calculation, that the cutoff-dependent terms are related to the geometry of the problem under consideration. Thus the coefficient of the ω_0^2 term is shown to be proportional to the total boundary length, while the coefficient of the $\ln\omega_0 R$ term is proportional to $\int |c(s)|^2\,ds$, where $c(s)$ represent the curvature of the boundary at the point s. These results make it clear that the divergences present in the expression for the Casimir energy cannot be eliminated by local subtractions, i.e.,[8] by renormalizing the parameters of the scalar field alone. It is, however, possible to argue that for the system consisting of the scalar field plus a region inside a boundary the parameter of the scalar field and the parameters of the boundary must both be renormalized when one eventually constructs a quantum theory for such a system. Finally there is an appendix in which a sketch of Pleijel's[9] result relating the asymptotic behavior of a certain integral of a Green's function to geometry, which we use to obtain the result of Sec. V, is given.

II. THE GREEN'S FUNCTION METHOD[3,4]

The method we use is standard.[3,4] A quick review is included for the sake of completeness. Consider the following Green's function in a region Γ:

$$\left(\frac{\partial^2}{\partial t_x^2} - \nabla_x^2\right)G_+(\mathbf{x},\mathbf{y};\tau) = \delta^D(\mathbf{x}-\mathbf{y})\delta(\tau), \tag{2.1}$$

where $\tau = t_x - t_y$, $\mathbf{x} = (x_1, x_2, \ldots, x_D)$,

$\mathbf{y} = (y_1, y_2, \ldots, y_D)$, $\delta^D(\mathbf{x}) \equiv \delta(x_1)\delta(x_2)\cdots\delta(x_D)$

and $\mathbf{x},\mathbf{y}\in\Gamma$. Writing

$$G_+(\mathbf{x},\mathbf{y},\tau) = \int_{-\infty}^{+\infty}\frac{dw}{2\pi}\,e^{iw\tau}G_+(\mathbf{x},\mathbf{y},\omega), \tag{2.2}$$

we get

$$[-\nabla^2 - \omega^2]G_+(\mathbf{x},\mathbf{y},\omega) = \delta^D(\mathbf{x}-\mathbf{y}). \tag{2.3}$$

If we introduce

$$-\nabla^2 U_n(\mathbf{x}) = \omega_n^2 U_n(\mathbf{x}), \tag{2.4}$$

where

$$U_n(\mathbf{x}) = 0, \quad \text{when } \mathbf{x}\in\partial\Gamma,$$

the boundary of the region Γ and

$$\int U_n^*(\mathbf{x})U_m(\mathbf{x})\,d^D x = \delta nm, \tag{2.5}$$

$$\sum_n U_n^*(\mathbf{x})U_m(\mathbf{y}) = \delta^D(\mathbf{x}-\mathbf{y}). \tag{2.6}$$

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Then we have

$$\int d^{D}x\, G_{+}(\mathbf{x},\mathbf{x},\tau) = i\sum_{n}\frac{e^{i\omega_n\tau}}{2\omega_n}. \tag{2.7}$$

The expression on the right is obtained by choosing an appropriate contour of integration in the complex ω plane. This contour characterizes the Green's function G_{+}. Following Schwinger's[4,10] prescription for continuing to the Euclidean Green's function we get

$$E(\omega_0) = \sum(\tfrac{1}{2}\omega_n)e^{-\omega_n/\omega_0} = \int_0^{\infty}\frac{d\omega}{\pi}\,\omega^2 e^{-\omega_n/\omega_0}\int G_{+}(x,x,i\omega)\,d^{D}x. \tag{2.8}$$

This will be our tool for calculating the Casimir energy which will be defined to be the $\lim\omega_0\to\infty$ of $E(\omega_0)$.

III. THE CASE OF THE CIRCULAR BOUNDARY IN TWO SPATIAL DIMENSIONS

We now apply Eq. (2.8) to the case of a circular boundary in two spatial dimensions. For a circular boundary it is convenient to introduce polar coordinates (r,θ) so that the equation for $G_{+}(\mathbf{x},\mathbf{y},\omega)$ becomes

$$\left\{-\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}\right]-\omega^2\right\}G_{+}(\mathbf{x},\mathbf{y},\omega) = \frac{1}{r}\delta(r-r')\delta(\theta-\theta'). \tag{3.1}$$

Writing

$$G(\mathbf{x},\mathbf{y},\omega) = \sum_{n=-\infty}^{+\infty} g_n(r,r')e^{in(\theta-\theta')},$$
$$\delta(\theta-\theta') = \sum_{n=-\infty}^{+\infty}\frac{e^{in(\theta-\theta')}}{2\pi}, \tag{3.2}$$

the differential equation satisfied by $g_n(r,r')$ is found to be

$$\frac{d}{dr}\left[r\frac{d}{dr}g_n(r,r')\right]-(n^2-\omega^2r^2)\frac{1}{r}g_n(r,r') = -\frac{1}{2\pi}\delta(r-r'), \tag{3.3}$$

and $g_n(r,r')$ must satisfy the usual discontinuity condition $(\epsilon\to 0)$,

$$\left[r\frac{dg_n(r,r')}{dr}\right]_{r=r'+\epsilon}-\left[r\frac{dg_n(r,r')}{dr}\right]_{r=r'-\epsilon} = (-)\frac{1}{2\pi}. \tag{3.4}$$

There are two regions to consider in our problem. Region I where $0\leqslant r\leqslant R$ and Region II, here $R\leqslant r\leqslant\infty$. In Region I, $g_n^{\mathrm{I}}(r,r')$ is regular at $r=0$ and $g_n^{\mathrm{I}}(r,r')=0$ when $r=R$. From these boundary conditions and (3.4) we get

$$g_n^{\mathrm{I}}(r,r') = \begin{cases} -\frac{i}{4}J_n(r\omega)\left[\frac{H_n^{(1)}(R\omega)}{J_n(R\omega)}J_n(r'\omega)-H_n^{(1)}(r'\omega)\right], & r<r', \\ -\frac{i}{4}J_n(r'\omega)\left[\frac{H_n^{(1)}(R\omega)}{J_n(R\omega)}J_n(r\omega)-H_n^{(1)}(r\omega)\right], & r>r', \end{cases} \tag{3.5}$$

where $J_n(r)$ represents a Bessel function and $H_n^{(1)}(r)$ a Hankel function of the first kind. Choosing the Hankel function corresponds to the boundary conditions appropriate for the Green's function G_{+}. Similarly $g_n^{\mathrm{II}}(r,r')$ which vanishes when $r=R$ and is to lead to an outgoing wave for $G_{+}(x,y,\tau)$ is found to be

$$g_n^{\mathrm{II}}(r,r') = \begin{cases} -\frac{i}{4}H_n^{(1)}(r'\omega)\left[J_n(r\omega)-\frac{J_n(R\omega)}{H_n^{(1)}(R\omega)}H_n^{(1)}(r\omega)\right], & r<r', \\ -\frac{i}{4}H_n^{(1)}(r\omega)\left[J_n(r'\omega)-\frac{J_n(R\omega)}{H_n^{(1)}(R\omega)}H_n^{(1)}(r\omega)\right], & r>r'. \end{cases} \tag{3.6}$$

Finally we determine the Greens function $G^0(\mathbf{x},\mathbf{y},\omega)$ corresponding to the case when there is no circular boundary at $r=R$. The appropriate $g_n^0(r,r')$ is found to be

$$g_n^0(r,r') = \begin{cases} \frac{i}{4}J_n(r\omega)H_n^{(1)}(r'\omega) & r<r', \\ \frac{i}{4}J_n(r'\omega)H_n^{(1)}(r\omega) & r>r'. \end{cases} \tag{3.7}$$

The expression for the Casimir energy can now be written as

$$E(\omega_0) = \int_0^{\infty}\frac{d\omega}{\pi}e^{-\omega/\omega_0}\omega^2\sum_{n=-\infty}^{\infty}\int_0^{\infty}r\,dr \times\int_0^{2\pi}d\theta\,\tilde{g}_n(i\omega,r,r), \tag{3.8}$$

where

$$\tilde{g}_n \equiv (g_n^{\mathrm{I}}-g_n^0) \text{ in Region I} \equiv (g_n^{\mathrm{II}}-g_n^0) \text{ in Region II}$$

so that $E(\omega_0)\equiv 0$ when the circular boundary is absent. Substituting (3.5), (3.6), and (3.7) in (3.8), we get

$$E(\omega_0) = \int_0^{\infty}\frac{d\omega}{\pi}\omega^2e^{-\omega/\omega_0}\sum_{n=-\infty}^{+\infty}\int_0^{R}r\,dr \times\int_0^{2\pi}\left(\frac{-i}{4}\right)[J_n(i\omega r)]^2\cdot\frac{H_n^{(1)}(i\omega R)}{J_n(i\omega R)} + \int_R^{\infty}r\,dr\int_0^{2\pi}d\theta\left(\frac{-i}{4}\right)[H_n^{(1)}(i\omega r)]^2\cdot\frac{J_n(i\omega R)}{H_n^{(1)}(i\omega R)}. \tag{3.9}$$

Evaluating the integrals using results of the type

$$\int_0^{R}r\,dr\,J_n^2(\alpha r) = \tfrac{1}{2}R^2[J_n^2(\alpha R)-J_{n-1}(\alpha R)J_{n+1}(\alpha R)] \tag{3.10}$$

and making use of

$$J_{n-1}(x)+J_{n+1}(x) = \frac{2n}{x}J_n(x),$$
$$J_{n-1}(x)-J_{n+1}(x) = 2\frac{dJ_n}{dx} = 2J_n'(x), \tag{3.11}$$
$$H_n(x)J_n'(x)-J_n(x)H_n'(x) = \frac{2}{\pi ix},$$

we get

$$E(\omega_0) = (-)\frac{1}{2\pi R}\sum_{n=-\infty}^{+\infty}\int_0^\infty dy\, y e^{-y\epsilon} \times\left[\frac{I_n'(y)}{I_n(y)} + \frac{K_n'(y)}{K_n(y)}\right], \tag{3.12}$$

where $y = \omega R$, $\epsilon = 1/\omega_0 R$ and $I_n(x)$, $K_n(x)$ are the usual modified Bessel functions defined by

$$I_n(x) = e^{-n\pi i/2} J_n(ix), \qquad K_n(x) = \tfrac{1}{2}\pi i e^{n\pi i/2} H_n^{(1)}(ix). \tag{3.13}$$

Equation (3.12) is our final expression for the Casimir energy.

IV. NUMERICAL RESULTS

In this section we evaluate (3.12) in the limit $\epsilon \to 0$ (i.e., $\omega_0 \to \infty$). Making use of the fact that $I_{-n}(x) = I_n(x)$, $K_{-n}(x) = K_n(x)$, we can write (3.12) as

$$E(\epsilon) = (-1)\frac{1}{\pi R}\sum_{n=1}^{\infty}\int_0^\infty dy\cdot y\cdot e^{-y\epsilon} \times\left[\frac{I_n'(y)}{I_n(y)} + \frac{K_n'(y)}{K_n(y)}\right] + T_0, \tag{4.1}$$

where

$$T_0 = (-)\frac{1}{2\pi R}\int_0^\infty dy\cdot y\cdot e^{-y\epsilon}\left[\frac{I_0'(y)}{I_0(y)} + \frac{K_0'(y)}{K_0(y)}\right].$$

Integrating by parts, (4.1) can be written as

$$F(\epsilon) = (-)\frac{1}{\pi R}\sum_{n=1}^{\infty}\frac{1}{\epsilon}\int_0^\infty dx\, e^{-\epsilon n x} \times\frac{d}{dx}\left[x\frac{d}{dx}\ln I_n(nx)K_n(nx)\right] - \frac{1}{2\pi R}\int_0^\infty dx\cdot x\cdot e^{-\epsilon x}\frac{d}{dx}\cdot\ln I_0(x)K_0(x). \tag{4.2}$$

Using the uniform asymptotic expansions for $I_n(nx)$, $K_n(nx)$ given by (for large n)[1,4]

$$I_n(nx)K_n(nx) \sim \frac{1}{2n(1+x^2)^{1/2}}\left[1 + \frac{1}{n^2}(0.125t^2 - 0.75t^4 + 0.625t^6) + O\left(\frac{1}{n^3}\right) + \cdots\right], \tag{4.3}$$

where $t = 1/(1+x^2)^{1/2}$. We get for the contribution of the leading term of the expansion (4.3) to $E(\epsilon)$,

$$E^{(1)}(\epsilon) = \frac{1}{\pi R}\sum_{n=1}^{\infty}\frac{2}{\epsilon}\int_0^\infty dx\cdot\frac{x}{(1+x^2)^2}\cdot e^{-\epsilon n x}. \tag{4.4}$$

For the $n = 0$ term we use (for large x)[10]

$$I_0(x)K_0(x) \sim \frac{1}{2x} \tag{4.5}$$

to get the asymptotic contribution to T_0:

$$E^{(0)}(\epsilon) = \frac{1}{2\pi R}\int_0^\infty dx\cdot e^{-\epsilon x} = +\frac{1}{2\pi R}\frac{1}{\epsilon} \tag{4.6}$$

which is divergent as $\epsilon \to 0$.

Let us evaluate $E^{(1)}(\epsilon)$. The summation over n can be carried out to give

$$E^{(1)}(\epsilon) = \frac{1}{\pi R}\cdot\frac{2}{\epsilon}\int_0^\infty\frac{dx\cdot x}{(1+x^2)^2}\cdot\frac{1}{(1-e^{-\epsilon x})}.$$

Writing

$$\frac{1}{1-e^{-\epsilon x}} = \frac{e^{\epsilon x}}{\epsilon x}\left[1 - \tfrac{1}{2}(\epsilon x) + \tfrac{1}{12}(\epsilon x)^2 - \cdots\right],$$

we get

$$\lim_{\epsilon\to 0} E^{(1)}(\epsilon) = \frac{1}{\pi R}\cdot\left|\frac{\pi}{2}\cdot\frac{1}{\epsilon^2} - \frac{1}{2}\cdot\frac{1}{\epsilon} + \frac{\pi}{24}\right|. \tag{4.7}$$

It is interesting to note that the linearly divergent piece of $E^{(0)}(\epsilon)$ cancells the corresponding term of $E^{(1)}(\epsilon)$. In Sec. V we will see that this cancellation can be understood from the geometry of the problem.

We next evaluate numerically a few terms of the series:

$$\lim_{\epsilon\to 0}[E(\epsilon) - E^{(1)}(\epsilon) - E^{(0)}(\epsilon)] = (-)\frac{1}{2R}\sum_{n=0}^{\infty}\frac{g}{\pi}\int_0^\infty dy\left[y\left\{\frac{I_n'(y)}{I_n(y)} + \frac{K_n'(y)}{K_n(y)}\right\} + \frac{y^2}{n^2+y^2}\right], \tag{4.8}$$

where we have set $\epsilon = 0$ inside the integral and

$$g = \begin{cases} 2, & n \neq 0, \\ 1, & n = 0. \end{cases}$$

Defining

$$F_n = \frac{g}{\pi}\int_0^\infty dy\left[y\left\{\frac{I_n'(y)}{I_n(y)} + \frac{K_n'(y)}{K_n(y)}\right\} + \frac{y^2}{n^2+y^2}\right], \tag{4.9}$$

we find

$$F_0 = 0.02925, \quad F_1 = 0.01564, \quad F_2 = 0.00782, \quad F_5 = 0.0057. \tag{4.10}$$

We also evaluate the next to leading asymptotic contribution of $E(\epsilon)$ by using Eq. (4.3). This means evaluating

$$E^{(2)} = +\frac{1}{\pi R}\sum_{n=1}^{\infty}\frac{1}{n}\int_0^\infty dy\cdot y\cdot[2\times 0.125y/(1+y^2)^2] - \frac{4\times 0.75y}{(1+y^2)^3} + \frac{0.625y\times 6}{(1+y^2)^4} \equiv \frac{1}{2R}\sum_{n=1}^{\infty}F_n^{(1)},$$

$$F_n^{(1)} = \frac{1}{n}\int_0^\infty dy\cdot y\left[\frac{2\times 0.125y}{(1+y^2)^2} - \frac{4\times 0.75y}{(1+y^2)^3} + \frac{6\times 0.625y}{(1+y^2)^4}\right]. \tag{4.11}$$

We find that

$$F_n^{(1)} = \frac{0.01562}{n}. \tag{4.12}$$

Comparing $F_n^{(1)}$ for $n = 1$ and $n = 2$ with our numerical integration results (4.10), we find they are very similar. Equation

(4.12) also tells us that a more careful evaluation of $\lim_{\epsilon\to 0}[E(\epsilon)-E^{(1)}(\epsilon)]$ is necessary since $\Sigma_{n=1}^{\infty}F_n^{(1)}$ is a divergent quantity. In effect we should not set $\epsilon=0$ inside the integrals. We are thus led to evaluating

$$\tilde{F}=\lim_{\epsilon\to 0}[E(\epsilon)-E^{(1)}(\epsilon)]$$
$$=\frac{1}{2R}\left\{\frac{2}{\pi}\sum_{n=1}^{L}\frac{1}{n}\int_0^\infty dy\left[\frac{0.25y^2}{(1+y^2)^2}-\frac{3y^2}{(1+y^2)^3}+\frac{3.75y^2}{(1+y^2)^4}\right]+\frac{2}{\pi}\sum_{n=(L+1)}^{\infty}\frac{1}{n}\int_0^\infty dy\,e^{-n\epsilon y}\times\left[\frac{0.25y^2}{(1+y^2)^2}-\frac{3y^2}{(1+y^2)^3}+\frac{3.75y^2}{(1+y^2)^4}\right]\right\}. \quad (4.13)$$

Using the Euler–Maclaurin summation formula[10]

$$\sum_{L+1}^{\infty}f_n\cong\int_{L+1}^{\infty}f_n\,dn-\tfrac{1}{2}[f(L+1)+f(\infty)]+\cdots \quad (4.14)$$

and

$$\sum_{1}^{L}\frac{1}{n}=\gamma+\psi(L+1),\quad \gamma=0.577\cdots,$$

where $\psi(L)$ is the Digamma function which has the property that for large L [11]

$$\psi(L)\sim\ln L-\frac{1}{2L}-\frac{1}{12L^2}+\cdots,$$

we get

$$\tilde{F}=(-)\frac{1}{2R}\cdot\left[\frac{1}{64}\right][\gamma+\ln\omega_0R]. \quad (4.15)$$

Writing $(L+1)=\omega_0R$, all the contribution to $\tilde{F}$ comes from the first term of Eq. (4.13). The integral term does not cancel the divergent term. This is most easily seen if we note that for large L,

$$\int_{L+1}^{\infty}\frac{e^{-n\epsilon x}}{n}dn\sim\frac{e^{-(L+1)}}{L+1}\left[1-\frac{1}{(L+1)}+\frac{2}{(L+1)^2}-\cdots\right]. \quad (4.16)$$

Thus our final expression for the Casimir energy, to at least two decimal place accuracy for the finite piece, is

$$E(\omega_0)=+\frac{1}{2R}\times 0.045-\frac{1}{128R}\ln\omega_0R+\frac{R}{2}\omega_0^2. \quad (4.17)$$

$E(\omega_0)$ for our two-dimensional problem appears to be cut-off dependent unlike the result of Milton, DeRaad, and Schwinger for the three-dimensional conducting shell in an electromagnetic field.[12] We turn to a discussion of the divergent piece of Eq. (4.17) in the next section.

V. DIVERGENT TERMS AND GEOMETRY

In the previous section the Casimir energy was evaluated and found to contain cutoff (ω_0)-dependent terms. It might be argued that these terms would not arise if Eq. (2.8) were properly evaluated. We will now show that this is not the case. If we accept Eq. (2.8) as a proper starting point for calculating the Casimir energy $E(\omega_0)$ then certain types of cutoff-dependent terms must be present. In order to be very general we consider the case of a two-spatial-dimensional region with an arbitrary smooth boundary. It is further required that the region be compact. Under these circumstances Pleijel[9] showed in 1954 that for large ω,

$$\int d^2x\tilde{G}(\mathbf{x},\mathbf{x},i\omega)\sim\frac{1}{\omega}\cdot\frac{S}{8}-\left[\frac{1}{12\pi}\int c(s)\,ds\right]\frac{1}{\omega^2}-\frac{1}{\omega^3}\left[\frac{1}{512}\int c^2(s)\,ds\right]+\cdots. \quad (5.1)$$

where S is the length of the smooth boundary an arbitrary point of which is located by means of s the arc length of the point from a fixed point on the boundary, $c(s)$ is the curvature of the boundary at the point s and $\tilde{G}_+=G_+-G_0$. A sketch of the way (5.1) may be derived is given in the Appendix. Clearly Eq. (5.1) is exactly what we need to discuss the divergences of $E(\omega_0)$ as $\omega_0\to\infty$.

We recall that

$$E(\omega_0)=\int_0^\infty\frac{d\omega}{\pi}\cdot\omega^2e^{-\omega/\omega_0}\int\tilde{G}_+(\mathbf{x},\mathbf{x},i\omega)\,d^Dx. \quad (5.2)$$

Substituting (5.1) in (5.2) we get

$$E(\omega_0)=\frac{S}{8\pi}\cdot\omega_0^2-\left(\tfrac{1}{12}\int c(s)\,ds\right)\omega_0-\left(\tfrac{1}{512}\int c^2(s)\,ds\right)\times\ln\omega_0R+\text{finite part of }E(\omega_0). \quad (5.3)$$

In our problem there are two regions to consider. Thus the divergent terms of $E(\omega_0)$ in terms of geometrical factors are

$$E^{\infty}(\omega_0)=\frac{S}{4\pi}\omega_0^2-\left(\tfrac{1}{256}\int c^2(s)\,ds\right)\ln\omega_0R. \quad (5.4)$$

The coefficient of the ω_0 term is zero, since

$$\left(\int_{\mathrm{I}}c(s)\,ds+\int_{\mathrm{II}}c(s)\,ds\right)=0.$$

Subtituting $S=2\pi R$,

$$c(s)=1/R,\quad\int ds=\int_0^{2\pi}Rd\theta\ ,$$

we get

$$E^{\infty}(\omega_0)=[(R/2)\omega_0^2-(1/128R)\ln\omega_0R] \quad (5.5)$$

which agrees exactly with the result of Sec. IV. The presence of the cutoff-dependent terms in $E(\omega_0)$ can be viewed in at least two different ways. It can be argued that the boundary condition $U_n(\mathbf{x})=0$ for all ω_n is physically unrealistic. Real boundaries become transparent for large frequencies. Thus the parameter ω_0 introduced in our calculations really represents a physical quantity. Given the composition of the boundary and the way it interacts [in our case with the scalar field $\phi(\mathbf{x},t)$] one should be able to calculate ω_0. Once ω_0, for a particular boundary, is determined our expression for the Casimir energy is no longer ambiguous but represent the physically measurable zero-point energy of the system. Namely, that

$$E(\omega_0)=+\frac{0.045}{2R}+\left[\frac{R}{2}\omega_0^2-\frac{1}{128R}\ln\omega_0R\right]. \quad (5.6)$$

If in Eq. (5.6) we ignore the constant force the $(R^2/2)\omega_0^2$ term gives rise to, then Eq. (5.6) implies a change in the sign of the Casimir force in the neighborhood of a critical radius R_c

defined by $\omega_0 R_c \tilde{=} 48.42$. When $R > R_c$, the force is attractive while for $R < R_c$ the force becomes repulsive. (Remember ω_0 is not a variable.) A very intriguing state of affairs.

Alternatively one can argue that the cut-off dependent terms are telling us that the "bare" parameters of the extended object we are considering have to be renormalized. The system being considered consists of the scalar field $\phi(\mathbf{x},t)$ and a region enclosed by the smooth boundary $\partial\Gamma$. Schematically we might expect the energy of the system to have the following structure:

$$E_{\text{total}} = E_{\text{field}} + E_{\text{boundary}}, \tag{5.7}$$

with

$$E_{\text{boundary}} = \alpha S'_R + \beta c_R(s)\,ds + \gamma c_R^2(s)\,ds + \cdots, \tag{5.8}$$

where S'_R = length of the boundary, $c_R(s)$ the curvature of the boundary,and $\alpha, \beta, \gamma, \ldots$ are numbers. The subscript R indicates that in general we might expect to have to renormalize the "bare boundary" parameters. For instance, we might have to write

$$c_R^2(s) \cong [1 - 0.35 \ln(\omega_0/m)](1/R^2), \tag{5.9}$$

indicating that $c_R^2 = 1/R^2$, when $\omega_0 = m$. A procedure of this nature, with the quantitive S_R, $c_R(s)$, c_R^2, etc. identified as the observable parameters of the boundary, would lead to the observable, renormalized, Casimir energy E_R being finite and given by

$$E_R = +0.045/(2R). \tag{5.10}$$

We do not have a procedure for carrying out such a renormalization scheme in a systematic way and mention it only as a possibility.[13]

ACKNOWLEDGMENTS

I would like to thank S. Ciulli and T. Murphy for helping me check the $n = 0$ and $n = 1$ numerical integrations of Sec. IV on the computer.

APPENDIX

We will sketch now Pleijel's result

$$\int d^2x\, \tilde{G}(\mathbf{x},\mathbf{x},i) \sim \frac{1}{\omega}\frac{S}{8} - \frac{1}{\omega^2}\left[\frac{1}{12\pi}\int c(s)\,ds\right] - \frac{1}{\omega^3}\left[\frac{1}{512}\int c^2(s)\,ds\right] + \cdots, \tag{A1}$$

where S is the length of the boundary, $c(s)$ the curvature may be obtained. Our treatment is based on the paper of Stewartson and Waechter (Ref. 9) and is included for the sake of completeness. A sign error of Pleijel's is corrected in this paper. The mathematical problem we have to solve is the following:

Given

$$[-\nabla^2 + s^2]\tilde{G}(\mathbf{x},\mathbf{x},s) = 0 \tag{A2}$$

in a region Γ and $\tilde{G} = (-)G_0 = (+)(1/2\pi)K_0(SR)$ an $\partial\Gamma$, determine the asymptotic expansion for large s of

$$\bar{K}(s^2) = \int \tilde{G}(\mathbf{x},\mathbf{x},s)\,d\Omega \tag{A3}$$

$$= \sum_{n=1}^{N} a_n s^{-n}. \tag{A4}$$

$K_0(x)$ represents the usual modified Bessel functions. The procedure of Stewartson and Waechter is to choose rectangular coordinates Pxy where P is a typical point of the boundary $\partial\Gamma$, P_x is directed along the inward drawn normal to $\partial\Gamma$ and P_y along the tangent at P. On making the transformation $\xi = xs$, $\eta = ys$, where $\mathbf{x} \equiv (x,y)$ the function $\tilde{G}$ can be written as

$$\tilde{G}(\xi,\eta;\xi_0,0;s^2) = \frac{1}{2\pi}K_0\{[(\xi+\xi_0)^2 + \eta^2]\}^{1/2} + \frac{1}{2\pi^2}\int_{-\infty}^{\infty} d\eta_1 f(\eta_1,s)\frac{\partial K_0}{\partial \xi}(\xi,\eta;0,\eta_1), \tag{A5}$$

where the source point is taken to be $(\xi_0,0)$ and the function f is to be found from the condition that $\tilde{G} = G_0$ on $\partial\Gamma$, provided that terms which are exponentially small in s are neglected. Physically we can think of f as representing a distribution of dipoles on $\xi = 0$ whose strengths are to be suitably chosen. For a smooth boundary $\partial\Gamma$ the Serret–Frenet formula tell us that

$$x = \sum_{n=2}^{\infty} \alpha_n y^n, \tag{A6}$$

where

$$\alpha_2 = K(\tau)/2, \quad \alpha_3 = K'(\tau)/6,$$
$$\alpha_4 = K''(\tau)/24 + (K^3/8), \text{ etc.},$$

$K(\tau)$ being the curvature of P, $K'(\tau)$ the derivative of the curvature of P with respect to the arc length τ, etc. In terms of ξ,η the equation for 2Γ becomes

$$\xi = \sum_{n=2}^{\infty} \frac{\alpha n}{s^{n-1}}\eta^n. \tag{A7}$$

An asymptotic determination $\tilde{G}$ can now proceed by writing

$$f(\eta,s) = \sum_n \frac{fn(\eta)}{s^n}. \tag{A8}$$

Once $\tilde{G}$ is determined $\bar{K}(s^2)$ can be written as

$$\int_{\partial\Gamma} d\tau \int_0^{\infty} \frac{d\xi_0}{S}\tilde{G}(\xi_0,0;\xi_0,0;s^2)\left[1 - \frac{K\xi_0}{S}\right], \tag{A9}$$

provided that terms which are exponentially small in terms of s are neglected.

To illustrate how the method works we calculate the coefficient of the $O(1/s^2)$ term [which is the same as the $O(1/\omega^2)$ coefficient].

It is found that

$$f_0(\eta,s) = +\frac{2\eta^2\xi_0}{(\xi_0^2+\eta^2)^{1/2}}K_0'[(\xi_0^2+\eta^2)^{1/2}].$$

Thus the $O(1/\omega^2)$ term of (A9) gets contribution from two terms:

$$\text{(i) } I_1 = (-)\int_{\partial\Gamma} d\tau \int_0^{\infty} d\xi_0\,(+2\alpha_2)\xi_0\left(\frac{1}{2\pi}\right)K_0(2\xi_0),$$

$$\text{(ii) } I_2 = \int \frac{\alpha_2}{2\pi^2}d\tau \int_{-\infty}^{\infty} f_0(\eta_1 s)\frac{\xi_0}{(\xi_0^2+\eta^2)^{1/2}} \times K_0'(\xi_0^2+\eta_1)\,d\eta_1.$$

Evaluating (i) gives

$$I_1 = \frac{1}{4\pi}\int_{\partial\Gamma} \alpha_2(\tau)\, d\tau.$$

To evaluate (ii) it is convenient to note that

$$K_0'(x) = (-)x\int_0^\infty \frac{dt}{4t^2} e^{-t-x^2/4t}.$$

Then we get

$$I_2 = (+)\int \frac{\alpha_2}{2\pi^2} d\tau \int_{-\infty}^{\infty} d\eta_1\, 2\eta_1^2 \times \int_0^\infty \frac{dt_1}{4t_1^2} \exp\left(-t_1 - \frac{(\xi_0^2+\eta_1^2)\infty}{4t_1}\right) \times \int_0^\infty \frac{dt_2}{4t_1^2} \exp\left(-t_2 - \frac{\xi_0^2+\eta_1^2}{t_2}\right).$$

Carrying out the ξ_0 integration first and introducing $T = t_1 + t_2$, $t = t_1 - t_2$, we get

$$I_1 = (+)\int \frac{\alpha_2}{2\pi^2}\cdot\frac{\pi}{4} d\tau \cdot \int_0^\infty dT \frac{e^{-T}}{T^3} \times \int_0^t \cdot (T-t)(T+t)\, dt = +\int_{\partial\Gamma} \frac{\alpha_2}{12\pi} d\tau,$$

so that

$$O(1/\omega)\text{coeff} = I_1 + I_2 = -\frac{1}{12\pi}\int_{\partial\Gamma} K(\tau)\, d\tau.$$

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Application of a stochastic waveguide propagation model to ocean acoustics

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(Received 21 October 1980; accepted for publication 20 July 1981)

The problem of interest is the long-range (low-frequency) propagation of acoustic signals through the ocean. The loss of spatial coherence of the signal as a result of scattering by large scale internal waves leads to a limitation on the resolution of the direction of the source of the signal. The applicability of a stochastic waveguide propagation model to this problem in ocean acoustics is investigated.

PACS numbers: 43.20.Mv, 43.20.Bi

I. INTRODUCTION

A problem of interest in acoustics and optics is the propagation of a wave through a randomly inhomogeneous waveguide. Previous research by Sutton and McCoy has led to a model applicable in both the single-scatter[1] and multiple-scatter[2] regions. The model is capable of including stochastically rough walls[3] as well as stochastical fluctuations in the index of refraction. In many problems of practical interest, e.g., in ocean acoustics, these index of refraction fluctuations have horizontal power spectra that follow a simple power law or a combination of such power laws. This paper investigates the application of the model to such problems.

II. FORMULATION OF PROPAGATION MODEL

Before considering the specific problem of interest it is worthwhile to look briefly at the formulation of the model. We will follow the development and notation used in Ref. 2.

The waveguide is referred to by Cartesian coordinates with the y axis directed normal to the waveguide plane, and the z axis is taken to correspond to the principal propagation direction. The acoustic medium is described by a weakly random sound speed field superimposed on a deterministic background field. The statistics of the fluctuating field are assumed to be homogeneous and isotropic for measurements taken in any given horizontal plane. The possibility of statistical inhomogeneity for measurements taken over the depth coordinate is retained, as is the possibility of statistical anisotropy for measurements taken over the depth coordinate when compared to those taken in a waveguide plane. The background sound speed field can vary with y but not with position in the waveguide plane. The acoustic field is taken to be harmonic in time with circular frequency ω.

The waveguide with the background medium is described by the normal mode functions, $Y_i(y)$, defined by the eigenvalue problem

$$\frac{d^2Y_i}{dy^2} + [\bar{k}^2(y) - \beta_i^2]Y_i = 0, \tag{1}$$

together with appropriate conditions at the waveguide face(s). The depth-dependent mean wavenumber is denoted by $\bar{k}^2 = \omega^2/\bar{c}^2$, where $\bar{c}(y)$ is the background sound speed field; the eigenvalue corresponding to the ith modal function is denoted by β_i.

The acoustic pressure field in the random waveguide problem, $\hat{p}(\mathbf{x})$, can be formally represented by

$$\hat{p}(\mathbf{x}) = \sum_i \hat{p}_i(\mathbf{r})Y_i(y). \tag{2}$$

The $\hat{p}_i(\mathbf{r})$ are termed the modal amplitudes and vary with position in the waveguide plane, located by the two-dimensional position vector $\mathbf{r}$. The modal amplitudes are governed by the set of differential equations,

$$\nabla_\perp^2\hat{p}_i + \beta_i^2\hat{p}_i = -\epsilon\sum_j \mu_{ij}(\mathbf{r})\hat{p}_j, \tag{3}$$

where

$$\mu_{ij}(\mathbf{r}) = \int \bar{k}^2(y)\mu(\mathbf{x})Y_i(y)Y_j(y)\,dy. \tag{4}$$

The two-dimensional Laplacian is denoted by $\nabla_\perp^2$, the randomly varying wavenumber field by $\epsilon\bar{k}^2(y)\mu(\mathbf{x})$. Here μ is a stochastic function of position of unit variance. Hence, ϵ provides a measure of the "strength" of the variations. We assume $\epsilon \ll 1$.

The theory is formulated in terms of modal coherence functions defined according to

$$\{\hat{\Gamma}_{ii}(x_1,x_2,z)\} = \{\hat{p}_i(x_1,z)\hat{p}_i^*(x_2,z)\}, \tag{5}$$

where the braces indicate an ensemble averaging. Thus, the coherence function is a spatial correlation function taken at two points in the same z plane. For an initial plane wave directed along the z axis and homogeneous statistics measured in the x, z plane, the modal coherence functions vary with $x_{12} = x_1 - x_2$ being independent of absolute position along the x axis.

The more familiar mutual coherence function for two points in the same z plane used extensively by McCoy and Beran[4,5] is given by

$$\{\hat{\Gamma}(x_1,y_1,x_2,y_2,z)\} = \{\hat{p}(x_1,y_1,z)\hat{p}^*(x_2,y_2,z)\}. \tag{6}$$

By substituting Eq. (2) into Eq. (6), we can write

$$\{\hat{\Gamma}(x_1,y_1,x_2,y_2,z)\} = \sum_i\sum_j\{\Gamma_{ij}(x_1,x_2,z)\}Y_i(y_1)Y_j(y_2), \tag{7}$$

where in writing Eq. (7) we were required to introduce cross-modal coherence functions, which are obvious generalizations of the $\{\hat{\Gamma}_{ii}\}$. Upon setting $y_1 = y_2$ in Eq. (7) and integrating over the waveguide depth, we obtain, upon making use of the orthonormality of the Y_i,

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$$\int \{\hat{\Gamma}(x_1,y,x_2,y,z)\}\, dy = \sum_i \{\hat{\Gamma}_{ii}(x_1,x_2,z)\}. \tag{8}$$

Equation (8) states that the modal coherence functions provide the modal decomposition of the averaged (taken over the waveguide depth) coherence for two points located along the same horizontal line positioned orthogonal to z.

In the range incrementing derivation procedure used in the formulation, the waveguide is divided by a series of range planes separated by a distance Δz. Since the problems to which the theory is to be applied involve only forward propagation, we then calculate the modal coherence functions at one range plane in terms of those of the plane immediately preceding it. The increment Δz is taken to be small enough to enable use of a single-scatter theory for this calculation. Also, in making this calculation, we assume the statistics of the $\hat{p}_i$ measured on any range plane to be independent of the statistics of the sound speed fluctuations in the interval "in front of" the range plane. This is clearly consistent with the forward propagation assumption over most of the interval if we take Δz to be large relative to l_{HM}, the maximum correlation length along a line in the horizontal plane. Finally, we make a series of approximations to simplify the single-scatter solution to a point at which computationally useful expressions are obtained. The result is a system of difference equations:

$$\{\hat{\Gamma}_{ii}(x_{12},(j+l)\Delta z)\} = \{\hat{\Gamma}_{ii}(x_{12},j\Delta z)\} - \epsilon^2\Big[\{\hat{\Gamma}_{ii}(x_{12},j\Delta z)\}\sum_k \bar{\sigma}_{ik}(0) - \frac{1}{\beta_i}\sum_k \beta_k \bar{\sigma}_{ik}(x_{12})\{\hat{\Gamma}_{kk}(x_{12},j\Delta z)\}\Big]\Delta z, \tag{9}$$

where $\bar{\sigma}_{ik}(x_{12})$ is defined in terms of the modal correlation matrix σ_{ikik}, which in turn is defined by the spatial correlation function σ of the randomly varying sound speed field and the modal eigenfunctions:

$$\bar{\sigma}_{ik}(x_{12}) = \frac{1}{2\beta_i\beta_k}\int_0^\infty \sigma_{ikik}(x_{12},s_z)\cos[(\beta_k-\beta_i)s_z]\, ds_z \quad (\text{note } s_z = z' - z''), \tag{10}$$

where

$$\sigma_{ijkl}(\mathbf{r}'-\mathbf{r}'') = \int\int \bar{k}^2(y')\bar{k}^2(y'')\sigma(\mathbf{x}',\mathbf{x}'')Y_i(y')Y_j(y')Y_k(y'')Y_l(y'')\times dy'dy'' \tag{11}$$

and

$$\sigma(\mathbf{x}',\mathbf{x}'') = \{\mu(\mathbf{x}')\mu(\mathbf{x}'')\}. \tag{12}$$

The set of difference equations can be approximated by a set of differential equations, which we write,

$$\frac{\partial\{\hat{\Gamma}_{ii}(x_{12},z)\}}{\partial z} = -\epsilon^2\Big(\sum_k \bar{\sigma}_{ik}(0)\Big)\{\hat{\Gamma}_{ii}(x_{12},z)\} + \frac{\epsilon^2}{\beta_i}\sum_k \beta_k\bar{\sigma}_{ik}(x_{12})\{\Gamma_{kk}(x_{12},z)\}. \tag{13}$$

The differential equations follow exactly from the difference equations in the limit of $\Delta z \to 0$. However, our derivation procedure requires $\Delta z \gg l_{\mathrm{HM}}$, where l_{HM} is the maximum correlation length along a line in the horizontal plane, making this final step an approximation. It is similar to the approximation taken in formulating a continuum theory to predict the response of a discrete system. Equation (13) is the equation governing the propagation of the modal coherence functions. The restrictions on the theory are detailed in Ref. 2.

III. APPLICATION OF PROPAGATION MODEL

If we view the separation distance x_{12} as a parameter in Eq. (13), then the set of equations constitutes a set of constant coefficient ordinary differential equations. The general solution of the set of equations is given by a linear combination of solutions of the form

$$\{\hat{\Gamma}_{ii}(z;x_{12})\} = \frac{1}{\beta_i}\gamma_i(x_{12})\exp[-\epsilon^2 a(x_{12})z], \tag{14}$$

which upon substitution in Eqs. (13) gives an eigenvalue problem for a. We write the characteristic equation as

$$\left|\left[a(x_{12}) - \hat{\sigma}_i - \left[\sum_{l\neq i}\bar{\sigma}_{il}(0)\right]\right]\delta_{ik} + (1-\delta_{ik})\bar{\sigma}_{ik}(x_{12})\right| = 0, \tag{15}$$

where

$$\hat{\sigma}_i(x_{12}) = \bar{\sigma}_{ii}(0) - \bar{\sigma}_{ii}(x_{12}). \tag{16}$$

In general, Eq. (15) has N roots, N being equal to the number of propagating modes. We denote the roots by $a^{(u)}(x_{12})$ and assume them to be distinct. Nondistinct roots introduce no conceptual difficulties. Associated with each characteristic value $a^{(u)}(x_{12})$ is a characteristic vector $\gamma_i^{(u)}(x_{12})$ obtained in the usual manner. The symmetry of the $\bar{\sigma}_{ik}(x_{12})$ provides an orthogonality relationship for the characteristic vectors. We make their definition unique by a normalization prescription.

Two limiting propagation experiments can be identified, a coherence dominated limit, defined by the condition that $(\hat{\sigma}_i - \hat{\sigma}_j) \gg \bar{\sigma}_{ij}^2$, and a modal intensity distribution dominated limit, defined by the reverse condition that $(\hat{\sigma}_i - \hat{\sigma}_j)^2 \ll \bar{\sigma}_{ij}^2$. In the ocean acoustics problem with which this paper is concerned the separation distances x_{12} of practical interest are large, and it is the coherence limit that is relevant. For a coherence dominated limit, the determinant of Eq. (15) is approximated by one that is diagonal, leading to characteristic values

$$a^{(u)}(x_{12}) = \bar{\sigma}_{uu}(0) - \bar{\sigma}_{uu}(x_{12}) + \sum_{l\neq u}\bar{\sigma}_{ul}(0), \tag{17}$$

and characteristic vectors

$$\gamma_i^{(u)}(x_{12}) = \delta_{iu}. \tag{18}$$

The first term on the rhs of Eq. (17) gives the rate of intramodal scatter, scatter from the μ mode; the second gives the separation distance over which this intramodal scatter correlates; the third gives the rate of intermodal scatter out of the μ mode. The first two terms are obtained for an uncoupled mode theory. The third term can be interpreted in terms of an apparent dissipation mechanism in that in this limit of large separation distances the intermodal scatter does not

correlate.

In ocean acoustics the problem of resolving the direction of the source of an acoustic signal is an important one, and it is known that the horizontal resolution limitation of an acoustic signal can be related to a characteristic distance defined by the transverse decay of the coherence function. At a particular z plane Eq. (14) shows that the modal coherence functions decay exponentially in the transverse direction according to the form $a(x_{12})$. Equation (17) gives the form of $a(x_{12})$ for the problem of interest in this paper. We need to evaluate $\bar{\sigma}_{ik}(x_{12})$.

Often a good approximation can be made to the spatial correlation function, $\sigma(\mathbf{x}',\mathbf{x}'')$, by the product $\sigma_H(\mathbf{r}',\mathbf{r}'')\sigma_V(y',y'')$, where $\sigma_H(\mathbf{r}',\mathbf{r}'')$ accounts for the horizontal and $\sigma_V(y',y'')$ the vertical fluctuations in the index of refraction.[6,7] For these situations it is seen from Eq. (11) that

$$\sigma_{ijkl}(\mathbf{r}'-\mathbf{r}'') = K_{ijkl}\sigma_H(\mathbf{r}'-\mathbf{r}'') \tag{19}$$

where

$$K_{ijkl} = \int_0^h \int_0^h \bar{k}^2(y')\bar{k}^2(y'')\sigma_V(y',y'') \times Y_i(y')Y_j(y')Y_k(y'')Y_l(y'')\,dy'dy'', \tag{20}$$

h being the depth of the waveguide.

It is convenient to discuss the horizontal fluctuations in the index of refraction in terms of the two-dimensional power spectrum $\phi(p,q)$. We write

$$\sigma_{ikik}(x_{12},s_z) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \phi(p,q)e^{-ips_z}e^{-iqx_{12}}\,dp\,dq. \tag{21}$$

Substituting for $\sigma_{ikik}(x_{12},s_z)$ in Eq. (10)and evaluating the integrals over s_z and p, we obtain

$$\bar{\sigma}_{ik}(x_{12}) = \frac{1}{2\beta_i\beta_k}\int_0^{\infty}\phi(\beta_k-\beta_i,q)\cos q\,x_{12}\,dq. \tag{22}$$

Now many problems of practical interest are concerned with index of refraction fluctuations that have horizontal power spectra that follow a simple power law or a combination of such power laws. It is well accepted among oceanographers that the most suitable description of the ocean temperature microstructure is in terms of a combination of power laws.[8] This is to be expected as different mechanisms cause the temperature fluctuations over different length scales. The longer size scale temperature fluctuations are due to the presence of randomly phased internal waves while the smaller scale temperature fluctuations are a result of ocean turbulence. Consequently, we will introduce the following specific form for the two-dimensional power spectrum

$$\phi(p,q) = \frac{A}{(q^2+p^2+c^2)^N}, \tag{23}$$

where A, c, and N are constants determined from oceanographic data. Equation (22) becomes

$$\bar{\sigma}_{ik}(x_{12}) = \frac{1}{2\beta_i\beta_k}\int_0^{\infty}\frac{A}{[q^2+(\beta_k-\beta_i)^2+c^2]^N} \times\cos q\,x_{12}\,dq. \tag{24}$$

This integral can be evaluated (see Gradshteyn and Ryzhik[9]). We obtain:

for $x_{12}\neq 0$,

$$\bar{\sigma}_{ik}(x_{12}) = \frac{A}{2\beta_i\beta_k\sqrt{\pi}}\left[\frac{2[(\beta_k-\beta_i)^2+c^2]^{1/2}}{x_{12}}\right]^{1/2-N} \times\cos(N-\tfrac{1}{2})\pi\Gamma(1-N) \times K_{N-1/2}(x_{12}[(\beta_k-\beta_i)^2+c^2]^{1/2}), \tag{25}$$

where Γ denotes the gamma function and K denotes a modified Bessel function;

for $x_{12}=0$,

$$\bar{\sigma}_{ik}(0) = \frac{A}{4\beta_i\beta_k}[(\beta_k-\beta_i)^2+c^2]^{1/2-N}\frac{\sqrt{\pi}\cdot\Gamma(N-\frac{1}{2})}{\Gamma(N)}. \tag{26}$$

Equations (17), (25), and (26) determine the detailed form of $a(x_{12})$ and consequently the transverse decay of the coherence function.

Although a combination of power laws is the most suitable description of the ocean temperature microstructure, often, for convenience, a single power law is used. For the length scales of interest in this paper (kilometers in the horizontal plane), there is general agreement that a minus two power law, $N=1$, is the most representative. For such a single power law we can write the following specific form for $a(x_{12})$:

$$a^i(x_{12}) = \frac{A\pi}{4\beta_i^2 c}(1-e^{-cx_{12}}) + \sum_{k\neq i}\frac{A\pi}{4\beta_i\beta_k}\cdot[(\beta_k-\beta_i)^2+c^2]^{-1/2}. \tag{27}$$

The modal coherence function decays to $1/e$ of its zero separation value at a distance l_Γ, called the characteristic transverse decay distance. l_Γ is determined by the following expression:

$$\epsilon^2 a^i(l_\Gamma^i)z = 1. \tag{28}$$

For the single power law representation we can write

$$l_\Gamma^i = \frac{1}{c}\ln\left\{1-4\beta_i^2\epsilon^{-2}cz^{-1}A^{-1}\pi^{-1} + \sum_{k\neq i}c\beta_i\beta_k^{-1}[(\beta_k-\beta_i)^2+c^2]^{-1/2}\right\}^{-1}. \tag{29}$$

For illustrative purposes consider an acoustic wave, frequency 50 Hz, propagating in a lossless waveguide of effective depth 25 m. Measured data[7,8] indicates that reasonable values for A, ϵ^2, and c are 10^{-2}, 10^{-7}, and 10^{-4}. Equation (29) shows that after propagating 50 km, the characteristic transverse decay distances for the two propagating modes are 209 and 1044 km.

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On approximating the solutions and critical points of some nonlinear phenomena

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(Received 23 March 1981; accepted for publication 26 June 1981)

We consider a nonlinear differential equation which arises in some heat transfer problems and study the applicability of Newton's method in approximating the physical solution. Also two methods are devised to approximate the physically interesting critical point, one based on the iterative method and the other on the Newton method. Using these methods, we obtain a sequence of linear-operator valued functions. The approximations are in the form of the fixed points of certain eigenvalues of the operators thus obtained. Some comments on numerical approximations of these fixed points are made.

PACS numbers: 44.90. + e, 02.30.Jr

1. INTRODUCTION

A considerable amount of attention has been paid to studying the differential equation[1-4]

$$-\nabla^2 u = \lambda f(u), \quad x \in D,$$
$$u(x) = 0, \quad x \in \partial D \tag{1}$$

which one encounters in some heat transfer problems[2] and the related problem of thermal explosion of gases.[4] Here $f(u) = f(x;u(x))$ is a nonlinear function of u and $x \in R^m, m \geqslant 1; \lambda$ is a real positive parameter; D is an open bounded subset of R^m and ∂D, the boundary of D, is piecewise continuous. From the physical viewpoint, the interest is in determining the critical value λ^* of the parameter λ defined by the condition that for each $\lambda < \lambda^*$ (1) has a positive solution and in obtaining the minimal solution $u(\lambda)$ for each such λ. A solution may or may not exist for $\lambda = \lambda^*$ depending on the properties of f.

As usual, we consider a more general equation (2) which is no more difficult to study than (1).

$$Lu = \lambda f(u), \quad x \in D$$
$$(Bu)(x) = \alpha(x)\, u(x) + \beta(x) \frac{\partial u(x)}{\partial \eta} = 0, \quad x \in \partial D, \tag{2}$$
$$\alpha(x) \geqslant 0, \not\equiv 0; \beta(x) \geqslant 0,$$

where L is the elliptic operator defined by

$$(Lu)(x) = -\sum_{i,j=1}^{m} \frac{\partial}{\partial x_i}\left(a_{ij}(x) \frac{\partial u(x)}{\partial x_j}\right) + a_0(x)u(x) \tag{3}$$

with the coefficients $a_{ij}(x)$ being the elements of a continuously differentiable matrix valued function on D which is bounded below by a positive constant; $a_0(x) \geqslant 0$ is continuous and $\partial/\partial\eta$ is the conormal derivative.[2] The function $f(x;\phi)$ will be assumed to satisfy conditions (i) to (iii):

(i) $f(x;\phi)$ is continuous for $x \in D$, $\phi \geqslant 0$,

(ii) $f(x;0) = f_0(x) > 0$ on D,

(iii) The derivative $f'(x;\phi)$ with respect to ϕ of $f(x;\phi)$ is continuous and positive on D for $\phi > 0$.

If $f'(\phi) = f'(\psi)$ for each $\phi \neq \psi$ then, clearly f is linear in ϕ. If $f'(\phi)$ is greater (less) than $f'(\psi)$ for $\phi > \psi \geqslant 0$, then f is called convex (concave). Some of the results depend on whether f is convex or concave.

Let $\mathscr{L}^2(D,dx)$ be the real Hilbert space of the square integrable functions with respect to the Lebesgue measure dx on D. Consider L as an operator from $\mathscr{D}(L)$ to $\mathscr{L}^2(D,dx)$, where

$$\mathscr{D}(L) = \left\{\{\phi: \frac{\partial^2 \phi(x)}{\partial x_i \partial x_j} \text{ is continuous, } x \in D;\right.$$
$$\left. i,j \leqslant m; (B\phi)(x) = 0, x \in \partial D\right\} \subset \mathscr{L}^2(D,dx).$$

In case the closure in $\mathscr{L}^2(D,dx)$ of L properly contains it, L will denote the closure. So defined, L is linear, self-adjoint, and bounded below by a positive constant. Therefore L^{-1} exists as a bounded operator and $L^{-1/2}$ is well defined. Let $f'(v)$ be the operation of multiplication by $f'(x;v(x))$ and $A(v) = L^{-1/2} f'(v) L^{-1/2}$; $A(v)$ for $v \geqslant 0$ is non-negative, bounded, and self-adjoint. Furthermore L^{-1} is a Hilbert–Schmidt operator which implies the same for $A(v)$ if v is bounded. Let the largest eigenvalue of $A(v)$ be $\gamma(v)$ and $\bar{\mu}(v) = 1/\gamma(v)$. Also let $u(\lambda)$ be the minimal positive solution of (2) for $\lambda < \lambda^*$. Then $A(u(\lambda))$, in addition to having the above properties, is a uniformly continuous function of $\lambda \in (0,\lambda^*)$, which implies the continuity of $\mu(\lambda) = \bar{\mu}(u(\lambda))$. These properties follow trivially from the results contained in Ref. 2, where $\mu(\lambda)$ was introduced in a slightly different but equivalent manner. We find the present formulation more convenient for some of the analysis to follow, mainly in connection with approximating λ^*. Convergence of the approximations to $u(\lambda)$ will be found to be stronger than the one in $\mathscr{L}^2(D,dx)$; therefore its Hilbert space structure is irrelevant for this purpose. The scalar product and the norm in $\mathscr{L}^2(D,dx)$ will be denoted by $(\cdot,\cdot)$ and $||\cdot||$, respectively.

With f satisfying conditions (i), (ii) and a milder monotonicity condition than (iii), the iterative procedure yields sequences which approximate $u(\lambda)$ from below for each $\lambda < \lambda^*$. But since the convergence of this method is usually poor, especially for λ close to λ^*, it is desirable to have better methods available. The Bubnov–Galerkin method[5] which is known to be very useful in solving linear problems,[5,6] reduces the present one to a finite set of nonlinear equations; and thus little is gained. Also when the solution is not unique it may be difficult to determine the minimal solution by this method. For these reasons the Newton method offers an attractive alternative for it reduces the problem to a succession

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of linear problems and when applicable, its convergence is considerably faster than the iterative method. However, the applicability of this method has been shown with severely restrictive conditions on f.[2,7] The most relevant results, for the present purpose, is the following: Let f be strictly concave, i.e., the second derivative $f''(\phi)$ of $f(\phi)$ be negative for $\phi > 0$, and $\lambda < \mu(0)$; then the Newton method approximates $u(\lambda)$ from above (Theorem 5.3, Ref. 2). It should be remarked that the strict concavity is not needed in the proof. Even then the result is of a limited value since λ^* in this case is strictly greater than $\mu(0)$. In the following, we improve upon this result to include each $\lambda < \lambda^*$. We show, further, that this method enables one to approximate $u(\lambda)$ from below for each $\lambda \leqslant \lambda^*$ even for a convex f. The convergence in both of the cases is uniform with respect to $x \in D \cup \partial D$. Some important nonlinearities in physical problems are convex, e.g., $f(x;\phi) = e^{\phi}$, as in the thermal explosion case.[4]

The problem of determining λ^* for a concave f reduces to solving a linear eigenvalue problem (Theorem 4.3, Ref. 2—see remark following Lemma 6 in the sequel). However, the same problem for a convex f has hardly been touched upon. Here we develop two methods to approximate λ^* from above in this case; one based on the iterative method and the other on Newton's method. The approximating sequence is in the form of the fixed points of certain approximations to an extension of $\mu(\lambda)$. The extended $\mu(\lambda)$ may be discontinuous at λ^* but the approximations are continuous. Parallel results follow for a concave f by trivial modifications in the arguments used for a convex f where the extended $\mu(\lambda)$ is continuous and the convergence is from below. However, since a more satisfactory method is available for this case, as mentioned above, the present method may not be preferable.

Some comments on approximating λ^* numerically are made in the concluding remarks.

2. PRELIMINARIES

In this section we collect some results to be used in the sequel, some of them repeatedly.

Lemma 1: Let ρ be the operation of multiplication by a positive continuous function $\rho(x)$ on D and $\phi \in \mathscr{D}(L)$. Also let $1/\tilde{\mu}$ be the largest eigenvalue of $L^{-1/2}\rho L^{-1/2}$.

(i) (Positivity lemma) Let $L\phi - \lambda\rho\phi > 0$ on D. Then $\phi(x) > 0$ on D if and only if $\lambda < \tilde{\mu}$.

(ii) (Weak positivity lemma) Let $L\phi - \lambda\rho\phi \geqslant 0$ on D and $\lambda < \tilde{\mu}$. Then $\phi(x) \geqslant 0$ on D.

For a proof of Lemma 1 see, for example, Ref. 2. Another proof of the sufficiency part of Lemma 1 (i) and that of (ii) may also be based upon the fact that the Green's function $G_\rho(x;\xi)$ corresponding to $(L - \lambda\rho)$ for $\lambda < \tilde{\mu}$ is positive.[8] Consequently the map $[L - \lambda\rho]^{-1}$ given by

$$w(x) = ([L - \lambda\rho]^{-1}v)(x) = \int_D d\xi\, G_\rho(x;\xi)v(\xi) \tag{4}$$

preserves positivity, which implies that it preserves also the monotonicity property of a sequence. In Lemma 2 and Corollary 1 we show that $[L - \lambda\rho]^{-1}$ not only preserve continuity, but also improves upon it.

Lemma 2: Let $L,\rho,\tilde{\mu}$ be as in Lemma 1 and $\lambda < \tilde{\mu}$. Also let $\{\phi_n\}$ be uniformly bounded and $\phi_n \underset{n\to\infty}{\to} \phi$ pointwise. Then $\psi_n = [L - \lambda\rho]^{-1}\phi_n \to_{n\to\infty} \psi = [L - \lambda\rho]^{-1}\phi$ uniformly with respect to $x \in D$, assuming further that $\{\psi_n\}$ is monotonic.

Proof: Consider

$$\lim_{n\to\infty} \psi_n(x) = \lim_{n\to\infty} \int_D d\xi\, G_\rho(x,\xi)\phi_n(\xi). \tag{5}$$

Since $\{\phi_n\}$ is uniformly bounded and $G_\rho(x;\xi)$ is a positive integrable function of $\xi \in D$, the integrand in (5) is bounded by an integrable function. Therefore, by the Lebesgue dominated convergence theorem, the order of limit and integral is interchangeable. Thus $\lim_{n\to\infty} \psi_n(x) = \psi(x)$ exists and clearly $\psi = [L - \lambda\rho]^{-1}\phi$. Also, from (5), $\psi(x)$ is continuous as is $\psi_n(x)$ for each n. Hence the convergence is uniform with respect to $x \in D$.

The following result, Corollary 1, may be obtained independently in a similar manner as the result of Lemma 2 or may be deduced from it. Therefore we state it without a proof.

Corollary 1: Let $L,\rho,\tilde{\mu}$ be as in Lemma 1 and $\lambda < \tilde{\mu}$. Also let $\phi_\xi(x)$ be a pointwise continuous function of ξ. Then $\psi_\xi = [L - \lambda\rho]^{-1}\phi_\xi$ is a continous function of ξ. If ϕ_ξ is monotonic in ξ, then the continuity is also uniform with respect to $x \in D$.

Lemma 3: Let $v < w$ on D. Then for a convex $f, \bar{\mu}(v) > \bar{\mu}(w)$ and for a concave $f, \bar{\mu}(v) < \bar{\mu}(w)$.

Proof: For a convex $f, v < w$ implies that $f'(v) < f'(w)$. Consequently for each $\phi \in \mathscr{L}^2(D,dx), (\phi, A(v)\phi) = (\phi, L^{-1/2}f'(v)L^{-1/2}\phi) < (\phi, L^{-1/2}f'(w)L^{-1/2}\phi) = (\phi, A(w)\phi)$ for $L^{-1/2}\phi \neq 0$. This implies the result. For a concave f, the inequality is clearly reversed.

In the following $u = u(\lambda) = u(x;\lambda)$ will denote the minimal positive solution of $Lu - \lambda f(u) = 0$, whenever it exists. With v being an initial approximation, Newton's approximation $w = \chi(v)$ is given by

$$w = \chi(v) = \lambda\,[L - \lambda f'(v)]^{-1}[f(v) - vf'(v)]. \tag{6}$$

It is clear that w is defined for $\lambda < \bar{\mu}(v)$. Also for a convex f, $\lambda < \lambda^*$ implies that $\mu(\lambda) > \lambda^*$ and $\mu(\lambda^*) = \lim_{\lambda \uparrow \lambda^*} \mu(\lambda) \geqslant \lambda^*$; while in case of a concave $f, \lambda < \mu(\lambda) < \lambda^*$ for $\lambda < \lambda^*$ which implies that $\mu(\lambda^*) = \lambda^*$ (Corollary 4.1.1 and 4.1.2 of Ref. 2). We have

Lemma 4: Let u,v,w be as above. Then

(i) For a convex $f, 0 \leqslant v < u$ implies that $w < u$ for each $\lambda \leqslant \lambda^*$.

(ii) For a concave $f, v > u$ implies that $w > u$ for $\lambda < \lambda^*$.

Proof: We have that

$$[L - \lambda f'(v)](u - w) = \lambda\,[f(u) - f(v) - (u - v)f'(v)] = \lambda\theta(u;v).$$

Convexity of f together with $v < u$ implies that $\theta(u;v) > 0$. Also from Lemma 3, $\bar{\mu}(v) > \bar{\mu}(u) = \mu(\lambda) \geqslant \lambda^* > \lambda$. The result now follows from Lemma 1 (i). For a concave f the argument is similar except that here $\bar{\mu}(v) > \bar{\mu}(u) = \mu(\lambda) > \lambda$ for $\lambda < \lambda^*$.

For a fixed λ, let $u_0(\lambda)$ be given and

$u_{n+1}(\lambda) = \chi(u_n(\lambda)), n = 0,1,2,\cdots$ The sequence $\{u_n(\lambda)\}$ will be called Newton's sequence generated by u_0.

Lemma 5: Let f be convex, $\lambda \leqslant \lambda^*$ and $\{u_n\}$ be Newton's sequence generated by $u_0(\lambda) = 0$. Then $u_n < u_{n+1} < u$ on D and all n.

Proof: If $u_n < u$ then from Lemma 4(i) $u_{n+1} < u$. Since $u_0 = 0 < u$, the induction principle yields that $\{u_n\}$ is bounded by u. Also from Lemma 3, $\lambda \leqslant \lambda^* \leqslant \bar{\mu}(u(\lambda)) < \bar{\mu}(u_n(\lambda))$.

Now, $u_1 = \lambda [L - \lambda f'(0)]^{-1} f(0)$ and $\lambda f(0) > 0$ on D. Hence from Lemma 1 (i) $u_1 > 0 = u_0$. Let $u_n > u_{n-1}$ on D. We have that

$$Lu_n = \lambda [f(u_{n-1}) + (u_n - u_{n-1}) f'(u_{n-1})] = \lambda \hat{\theta}(u_n; u_{n-1}).$$

Convexity of f together with $u_n > u_{n-1}$ implies that $\hat{\theta}(u_n; u_{n-1}) < f(u_n)$. Consequently

$$L(u_{n+1} - u_n) = \lambda [f(u_n) + (u_{n+1} - u_n) f'(u_n) - \hat{\theta}(u_n; u_{n-1})] > \lambda (u_{n+1} - u_n) f'(u_n),$$

i.e., $[L - \lambda f'(u_n)](u_{n+1} - u_n) > 0$ on D. We have already seen that $\lambda < \bar{\mu}(u_n)$ and hence from Lemma 1 (i), again, $u_{n+1} > u_n$ on D. By the induction principle it follows that $u_n < u_{n+1} < u$ for all n.

It should be remarked that, here and in the following, the strict monotonicity holds on D. On ∂D, $Bu_n = Bu = 0$ which could imply $u_n = u = 0$, e.g., if $\beta(x) = 0$. Also it is obvious that $u_n(\lambda) < u_{n+1}(\lambda)$ for each λ such that $\lambda < \bar{\mu}(u_n(\lambda))$. Setting $u(\lambda) = \infty$ for $\lambda > \lambda^*$, we have

Corollary 2: Let $\{u_n(\lambda)\}$ and $u(\lambda)$ be as above. Then $u_n(\lambda) < u_{n+1}(\lambda) < u(\lambda)$ for each λ such that $\lambda < \bar{\mu}(u_n(\lambda))$.

Lemma 6: Let f be concave, $\lambda < \lambda^*$ and $\{u_n\}$ be Newton's sequence generated by some $u_0 > u$. Then $u < u_{n+1} < u_n$ on D and all n.

Proof: Follows by an obvious transposition of the arguments of Lemma 5.

Remark: While the proof of Lemma 6 is straightfoward the condition $u_0 > u$ is rather stringent. If $\lim_{\phi \to \infty} [f(\phi) - \phi f'(\phi)] = F(x)$ exists then it is easy to check that $u_0 = \lambda [L - \lambda \bar{\rho}]^{-1} F$ will suffice where $\bar{\rho}(x) = \lim_{\phi \to \infty} f'(\phi)$. Since $f'(\phi)$ is a positive decreasing function of ϕ, $\bar{\rho}(x) \geqslant 0$ is well defined. It is claimed in Theorem 4.3 of Ref. 2 that $f(\phi) < \bar{F}(x) + \bar{\rho}(x)\phi$ with some $\bar{F}(x)$. If this were true for all concave f then, since $\bar{\rho}(x) \leqslant f'(\phi)$ and $[f(\phi) - \phi f'(\phi)]$ is an increasing function of ϕ, existence of the limit $F(x)$ would be guaranteed. But the inequality $f(\phi) < \bar{F}(x) + \bar{\rho}(x)\phi$ or even $f(\phi) < \bar{F}(x) + f'(\phi)\phi$ does not hold for an arbitrary concave f as can be easily seen by considering the example $f(x;\phi) = \ln(1 + x + \phi)$. Before we proceed to find a starting u_0, we comment on the result of Theorem 4.3 of Ref. 2.

The result in question is that λ^* is the reciprocal of the largest eigenvalue of $L^{-1/2} \bar{\rho} L^{-1/2}$, i.e., $\lambda^* = \bar{\mu}(\infty)$. The fact that $\lambda^* \leqslant \bar{\mu}(\infty)$ follows from the inequality $f(0) + \bar{\rho}\phi < f(\phi)$. The inequality $f(\phi) < \bar{F}(x) + \bar{\rho}(x)\phi$ was used to conclude that $\lambda^* \geqslant \bar{\mu}(\infty)$. It is obvious that, for each $\bar{\phi}, \phi$,

$$f(\phi) \leqslant [f(\bar{\phi}) - \bar{\phi} f'(\bar{\phi})] + \phi f'(\bar{\phi})$$

which implies that $\lambda^* \geqslant \bar{\mu}(\bar{\phi})$ (strict inequality is not needed in the proof of Theorem 3.3 of Ref. 2). Now, let $f'(\bar{\phi}) \to \bar{\rho}(x)$ uniformly on D as $\bar{\phi} \to \infty$. We have that

$$||A(\bar{\phi}) - A(\infty)|| \leqslant ||L^{-1/2}||^2 ||f'(\bar{\phi}) - \bar{\rho}|| \underset{\bar{\phi} \to \infty}{\to} 0$$

and hence $\lambda^* \geqslant \bar{\mu}(\infty) - \epsilon$. Here $\epsilon > 0$ can be chosen to be arbitrarily small by making $\bar{\phi}$ large. This is sufficient to conclude that $\lambda^* \geqslant \bar{\mu}(\infty)$.

If $F(x)$ as defined above exists then a convenient choice for u_0 is already given. The example $f(x;\phi) = x + \phi - e^{-\phi}$ shows that this method may be used for some concave nonlinearities. For the others, let κ be a positive constant such that $\lambda < \bar{\mu}(\kappa)$. Since $\bar{\mu}(\kappa)$ increases with κ and $\bar{\mu}(\infty) = \lambda^*$ for any $\lambda < \lambda^*$ a suitable κ may be found. Then $u_0 = \lambda [L - \lambda f'(\kappa)]^{-1} [f(\kappa) - \kappa f'(\kappa)]$ is defined. Since it is still true that

$$f(\phi) \leqslant [f(\kappa) - \kappa f'(\kappa)] + \phi f'(\kappa) \quad \text{for each } x \in D$$

it is easy to conclude that $u_0 \geqslant u$. But with this choice of u_0 the strict inequality of Newton's sequence may be lost and thus we have $u \leqslant u_{n+1} \leqslant u_n$ on D. However, this is inconsequential for the results to follow, for a strict inequality is not needed for the case of a concave f. We shall assume that a $u_0 > u$ has been found. If $u_0 \geqslant u$ is used then the modifications in the results are obvious. Since the present choices for u_0 appear to be the most suitable ones for computational purposes, we shall not consider others.

Lemma 7: Let f be convex and $\{\phi_n\}$ be a nondecreasing sequence of positive, continuous functions on D such that $\phi_n(x) \underset{n \to \infty}{\to} \infty$. Then $\lim_{n \to \infty} \bar{\mu}(\phi_n) = \bar{\mu}(\infty) \leqslant \lambda^*$.

Proof: As in Lemma 3 it is clear that $\{\bar{\mu}(\phi_n)\}$ is nonincreasing positive sequence. Hence $\lim_{n \to \infty} \bar{\mu}(\phi_n) = \bar{\mu}(\infty) \geqslant 0$ exists. Now, for each $\phi > 0$,

$$f(\phi) < f(0) + \phi f'(\phi) < f(0) + \phi f'(\infty)$$

implying that $\bar{\mu}(\infty) \leqslant \lambda^*$.

It should be remarked that if $f'(\infty) = \infty$ on a set of positive measure in D then $\bar{\mu}(\infty) = 0$.

3. APPROXIMATIONS TO $u(\lambda)$ AND λ^*

With the results of the last section available, convergence of Newton's sequence to $u(\lambda)$ in both of the cases is obtained in a straightforward manner.

Theorem 1: (i) Let f be convex, $\lambda \leqslant \lambda^*$ and $\{u_n(\lambda)\}$ be Newton's sequence generated by $u_0(\lambda) = 0$. Then $u_n \uparrow u$ uniformly with respect to x.

(ii) Let f be concave, $\lambda < \lambda^*$ and $\{u_n(\lambda)\}$ be Newton's sequence generated by $u_0(\lambda)$ of Lemma 6. Then $u_n \downarrow u$ uniformly with respect to x.

Proof: We give a proof here for (i). (ii) follows similarly by invoking Lemma 6 instead of Lemma 5 and noticing that in this case u is unique.

From Lemma 5, $\{u_n\}$ is an increasing sequence bounded by u and hence must converge pointwise from below to some $\bar{u} \leqslant u$. Further, we have that

$$Lu_n = \lambda \hat{\theta}(u_n; u_{n-1})$$

and $\hat{\theta}(u_n; u_{n-1}) \underset{n\to\infty}{\to} \lambda f(\bar{u})$ pointwise. Hence from Lemma 2, by setting $\rho = 0$, we have that $\bar{u} = \lim_{n\to\infty} u_n = \lambda L^{-1} f(\bar{u})$, i.e., $L\bar{u} = \lambda f(\bar{u})$; and the convergence is uniform. Since u is the minimal solution and $\bar{u} \leqslant u$ we must have $\bar{u} = u$.

In the following we obtain methods to approximate λ^*. We concentrate on the case of a convex f. It is trivial to modify the results and arguments for the case of a concave f, upon which we comment briefly.

The iterative method to approximate $u(\lambda)$ generates a sequence $\{v_n\}$ as follows: Let $v_0(\lambda) = 0$, $v_{n+1} = \lambda L^{-1} f(v_n)$, $n = 0,1,2,\cdots$. The sequence $\{v_n(\lambda)\}$ is clearly defined for all $\lambda \geqslant 0$ but it converges only for $\lambda < \lambda^*$. For a convex f, it may converge also for $\lambda = \lambda^*$. When convergent, $v_n(\lambda) \uparrow u(\lambda)$ uniformly with respect to $x \in D$.[2] Before we obtain approximations to λ^*, we have

Lemma 8: Let f be convex and $\mu_n(\lambda) = \bar{\mu}(v_n(\lambda))$. Then

(i) For each $n \geqslant 1$, $\mu_n(\lambda)$ is positive, continuous, and decreasing function of $\lambda \in (0,\infty)$; and $\mu_n(0) = \mu_0(\lambda) = \text{const} > 0$.

(ii) For each $\lambda \in (0,\infty)$, $\mu_n(\lambda) > \mu_{n+1}(\lambda) > \mu(\lambda)$ where $\mu(\lambda) = \mu(u(\lambda))$ for $\lambda \leqslant \lambda^*$ and $\mu(\lambda) = \bar{\mu}(\infty)$ for $\lambda > \lambda^*$).

Remark: For a concave f, $\mu_n(\lambda) < \mu(\lambda)$ increases with λ and $\mu_n(\lambda) \leqslant$ const. These extensions of $\mu(\lambda)$ have been obtained previously.[2] Here they will arise as limits of $\mu_n(\lambda)$ in a natural manner.

Proof: From Lemma 1 (i), $v_1(\lambda) = \lambda L^{-1} f(0)$ is positive. It is also a continuous and increasing function of $\lambda \in (0,\infty)$. Let this be true for $v_n(\lambda)$. Then from Corollary 1, $v_{n+1}(\lambda) = \lambda L^{-1} f(v_n(\lambda))$ is positive and continuous in λ. Further,

$$v_{n+1}(\lambda') - v_{n+1}(\lambda)$$
$$= (\lambda' - \lambda) L^{-1} f(v_n(\lambda')) + \lambda L^{-1}[f(v_n(\lambda')) - f(v_n(\lambda))]$$
$$> 0 \text{ for } \lambda' > \lambda \text{ [Lemma 1 (i)]}.$$

By the induction principle, $v_n(\lambda)$, for each n, is a positive, continuous, and increasing function of $\lambda \in (0,\infty)$. Let $A_n(\lambda) = A(v_n(\lambda)) = L^{-1/2} f'(v_n(\lambda)) L^{-1/2}$ and $\gamma_n(\lambda)$ be its largest eigenvalue. It follows that

(a) $A_n(\lambda)$ is positive, implying that $\gamma_n(\lambda)$ is positive.

(b) $A_n(\lambda)$ is a continuous function of $\lambda \in (0,\infty)$ in the uniform operator topology, i.e., $\lim_{\lambda \to \lambda'} ||A_n(\lambda) - A_n(\lambda')|| = 0$. This results in the continuity of $\gamma_n(\lambda)$.

(c) $A_n(\lambda)$ increases with λ, i.e., $(\phi, A_n(\lambda')\phi) > (\phi, A_n(\lambda)\phi)$ for $\lambda' > \lambda$ and each $\phi \in \mathscr{L}^2(D,dx)$. Hence $\gamma_n(\lambda)$ is an increasing function of λ.

(i) The first part of Lemma 8(i) follows from the fact that $\mu_n(\lambda) = 1/\gamma_n(\lambda)$. For the second part we observe that $v_n(0) = 0$ for each n and hence $A_n(0) = A(0)$ is independent of n, positive and bounded. Consequently $\mu_n(0) = \mu(0) = \text{const} > 0$.

(ii) We have that $\{v_n(\lambda)\}$ is monotonically increasing with n for each fixed λ, bounded above by $u(\lambda)$ where we set $u(\lambda) = \infty$ for $\lambda > \lambda^*$ (Theorem 3.2, Ref. 2). The result now follows from Lemma 3 and the fact that for $\lambda > \lambda^*$, $\mu(\lambda) = \mu(u(\lambda)) = \bar{\mu}(\infty)$ (Lemma 7).

Theorem 2: Let f be convex; then for each n, $\mu_n(\lambda)$ has a unique fixed point λ_n and $\lambda_n \downarrow \lambda^*$.

Remark: For a concave f, $\lambda_n \uparrow \lambda^*$.

Proof: Since $\mu_n(0) = \text{const} > 0$, and $\mu_n(\lambda)$ is a continuous and decreasing function of λ [Lemma 8 (i)], $\mu_n(\lambda)$ has a unique fixed point λ_n for each n. Thus $\{\lambda_n\}$ is well defined. [This result for concave f follows from the fact that $\mu_n(\lambda)$ increases with λ and is bounded by a constant.]

For $\lambda \leqslant \lambda^*$, from Lemma 8(ii) and Corollary 4.1.1 of Ref. 2, $\mu_n(\lambda) > \mu(\lambda) \geqslant \lambda^*$ and $\mu_n(\lambda) > 0$ for $\lambda > \lambda^*$. Also $\mu_n(\lambda)$ is continuous in λ; therefore $\lambda_n \geqslant \lambda^*$. Further, $\mu_n(\lambda)$ is decreasing with n and hence $\{\lambda_n\}$ is a decreasing sequence. Consequently $\lambda_n \downarrow \lambda_0^* \geqslant \lambda^*$. If $\lambda_0^* > \lambda^*$ then $\lambda_n \geqslant \lambda^* + \epsilon$ for all n and some $\epsilon > 0$. Hence $\mu_n(\lambda_n) \leqslant \mu_n(\lambda^* + \epsilon)$ for $\mu_n(\lambda)$ is a decreasing function of $\lambda \in (0,\infty)$ [Lemma 8(i)].

Now, $v_n(\lambda)$ of Lemma 8 increases without bound on D for $\lambda > \lambda^*$ and since $\mu_n(\lambda^* + \epsilon) = \bar{\mu}(v_n(\lambda^* + \epsilon))$, it follows from Lemma 7 that $\mu_n(\lambda^* + \epsilon) \underset{n\to\infty}{\to} \bar{\mu}(\infty)$. This implies that $\lim_{n\to\infty} \mu_n(\lambda_n) = \lim_{n\to\infty} \lambda_n \leqslant \bar{\mu}(\infty)$ but it is a contradiction for $\lambda_n > \lambda^* \geqslant \bar{\mu}(\infty)$. Consequently $\lambda_n \downarrow \lambda^*$.

In the following we give another method to approximate λ^* based on the Newton method. As in the case of $u(\lambda)$, this method should be expected to approximate λ^* better than the method of Theorem 2, but at the expense of increased computational labor to obtain each approximation. Thus, aside from being mathematically interesting, the above method may be better suited to solve some problems. Also some of the arguments used here will be found useful in the following.

Lemma 9: Let f be convex and $\nu_n(\lambda) = \bar{\mu}(u_n(\lambda))$, where $\{u_n(\lambda)\}$ is Newton's sequence generated by $u_0(\lambda) = 0$. Then for each $n \geqslant 1$ we have

(i) $\nu_n(\lambda)$ has a unique fixed point $\bar{\lambda}_n$ such that $\lambda^* < \bar{\lambda}_n < \bar{\lambda}_{n-1}$.

(ii) $u_n(\lambda)$ is positive, continuous, and increasing function of $\lambda \in (0,\bar{\lambda}_{n-1})$; $u_n(0) = 0$.

(iii) $\nu_n(\lambda)$ is positive, continuous, and decreasing for $\lambda \in (0,\bar{\lambda}_{n-1})$; $\nu_n(0) = \nu(0) = \text{const} > 0$.

Remark: For a concave f with $u_0(\lambda)$ as defined in Lemma 6, the inequalities are reversed.

Proof: The proof is by induction. It is clear that $\nu_0(\lambda) = \bar{\mu}(0) = \bar{\lambda}_0 > \lambda^*$. Since

$$u_1(\lambda) = \lambda [L - \lambda f'(0)]^{-1} f(0),$$

$u_1(0) = 0$, and the positivity of $u_1(\lambda)$ on $(0,\bar{\lambda}_0)$ follows from Lemma 1 (i). For the continuity and monotonicity we observe that for $\lambda < \lambda' < \bar{\lambda}_0$,

$$u_1(\lambda') - u_1(\lambda) = (\lambda' - \lambda)\{[L - \lambda' f'(0)]^{-1} f(0)$$
$$+ \lambda [L - \lambda' f'(0)]^{-1} f'(0)[L - \lambda f'(0)]^{-1} f(0)\} \downarrow 0$$

as $\lambda' \downarrow \lambda$ which is seen easily by using Lemma 1(i) and the boundedness of $[L - \lambda f'(0)]^{-1} f(0)$ for each $\lambda < \bar{\lambda}_0$. These properties of $u_1(\lambda)$ imply the properties stated in (iii) for $\nu_1(\lambda)$ exactly as in Lemma 8(i). Further, from Corollary 2, $0 = u_0(\lambda) < u_1(\lambda) < u(\lambda)$ for $\lambda \in (0,\bar{\lambda}_0)$ and hence

$\mu(\lambda) < \nu_1(\lambda) < \nu_0(\lambda)$ there from Lemma 3. It is clear that $\nu_1(0) = \bar{\lambda}_0$. These properties of $\nu_1(\lambda)$ imply that it has a unique fixed point $\bar{\lambda}_1$ such that $\lambda^* < \bar{\lambda}_1 < \bar{\lambda}_0$.

Assume (i)—(iii) to hold for n. For $(n+1)$ we have that

$$[L - \lambda f'(u_n(\lambda))]u_{n+1}(\lambda) = \lambda [f(u_n(\lambda)) - u_n(\lambda) f'(u_n(\lambda))], \quad (7)$$

i.e., $u_{n+1}(0) = 0$. By the induction assumptions (ii) and (iii) $u_n(\lambda), \nu_n(\lambda)$ are defined on $(0,\bar{\lambda}_{n-1})$ and since $\bar{\lambda}_n < \bar{\lambda}_{n-1}$ from (i), $(0,\bar{\lambda}_{n-1}) \supset (0,\bar{\lambda}_n)$. Thus $u_{n+1}(\lambda)$ is defined for $\lambda \in (0,\bar{\lambda}_n)$. Let $\lambda < \lambda' < \bar{\lambda}_n$.

$$\begin{aligned} L[u_{n+1}(\lambda') - u_{n+1}(\lambda)] &= \lambda' \hat{\theta}(u_{n+1}(\lambda');u_n(\lambda')) - \lambda \hat{\theta}(u_{n+1}(\lambda);u_n(\lambda)) \\ &= (\lambda' - \lambda)\hat{\theta}(u_{n+1}(\lambda');u_n(\lambda')) \\ &\quad + \lambda [\hat{\theta}(u_{n+1}(\lambda');u_n(\lambda')) - \hat{\theta}(u_{n+1}(\lambda);u_n(\lambda))] \\ &> \lambda [\hat{\theta}(u_{n+1}(\lambda');u_n(\lambda')) - \hat{\theta}(u_{n+1}(\lambda);u_n(\lambda))] \\ &= \lambda \eta(\lambda';\lambda). \end{aligned}$$

We have used the fact that

$$\hat{\theta}(u_{n+1}(\lambda');u_n(\lambda')) = f(u_n(\lambda')) + (u_{n+1}(\lambda') - u_n(\lambda'))f'(u_n(\lambda')) > 0$$

since $u_{n+1}(\lambda') > u_n(\lambda')$ for $\lambda' < \bar{\mu}(u_n(\lambda')) = \nu_n(\lambda')$ from Corollary 2. Since $\bar{\lambda}_n$ is the fixed point of $\nu_n(\lambda)$ as in (iii), $\lambda' < \nu_n(\lambda')$ for each $\lambda' < \bar{\lambda}_n$.

Further

$$\begin{aligned} \eta(\lambda',\lambda) &= [f(u_n(\lambda')) - f(u_n(\lambda)) - (u_n(\lambda') - u_n(\lambda))f'(u_n(\lambda))] \\ &\quad + [(u_{n+1}(\lambda') - u_n(\lambda'))(f'(u_n(\lambda')) - f'(u_n(\lambda)))] \\ &\quad + (u_{n+1}(\lambda') - u_{n+1}(\lambda))f'(u_n(\lambda)) \\ &> (u_{n+1}(\lambda') - u_{n+1}(\lambda))f'(u_n(\lambda)). \end{aligned}$$

Here we have used the convexity of f, the induction assumptions and Corollary 2. Thus

$$[L - \lambda f'(u_n(\lambda))]\,[u_{n+1}(\lambda') - u_{n+1}(\lambda)] > 0$$

and hence from Lemma 1(i), $u_{n+1}(\lambda') - u_{n+1}(\lambda) > 0$ for $\lambda < \nu_n(\lambda')$, i.e., for each $\lambda < \lambda' < \bar{\lambda}_n$. Positivity of $u_{n+1}(\lambda')$ follows from this by setting $\lambda = 0$. For the continuity we observe, following the above steps, that

$$u_{n+1}(\lambda') - u_{n+1}(\lambda) = [L - \lambda f'(u_n(\lambda))]^{-1}\bar{\eta}(\lambda';\lambda),$$

where for a fixed $(n+1)$, $\lim_{\lambda' \to \lambda} \bar{\eta}(\lambda';\lambda) = 0$. It is then straightforward to obtain, as in Lemma 2, that

$$\lim_{\lambda' \to \lambda}[u_{n+1}(\lambda') - u_{n+1}(\lambda)] = [L - \lambda f'(u_n(\lambda))]^{-1} \lim_{\lambda' \to \lambda} \bar{\eta}(\lambda';\lambda) = 0.$$

We have used the induction assumption that $u_n(\lambda)$ is continuous. Thus (ii) is established for $u_{n+1}(\lambda)$. This implies that $\nu_{n+1}(\lambda)$ is a positive, continuous, and decreasing function of $\lambda \in (0,\bar{\lambda}_n)$ from the same argument as in Lemma 8 (i).

Now, by Corollary 2,

$u(\lambda) > u_{n+1}(\lambda) > u_n(\lambda)$ for $\lambda \in (0,\bar{\lambda}_n)$ and hence $\mu(\lambda) < \nu_{n+1}(\lambda) < \nu_n(\lambda)$ from Lemma 3. This implies, as for $n = 1$, that $\nu_{n+1}(\lambda)$ has a unique fixed point $\bar{\lambda}_{n+1}$ such that $\lambda^* < \bar{\lambda}_{n+1} < \bar{\lambda}_n$.

Incidently, in proving Lemma 9, we have also obtained.

Corollary 3: Let the symbols be as in Lemma 9. Then for each n and $\lambda \in (0,\bar{\lambda}_{n-1})$,

(i) $u(\lambda) > u_n(\lambda) > u_{n-1}(\lambda)$, where $u(\lambda) = \infty$ for $\lambda > \lambda^*$,

(ii) $\mu(\lambda) < \nu_n(\lambda) < \nu_{n-1}(\lambda)$, where $\mu(\lambda) = \bar{\mu}(\infty)$ for $\lambda > \lambda^*$.

A counterpart of Corollary 2 is not required in order to obtain a result for concave f parallel to that of Lemma 9, for in that case $(0,\lambda^*) \supset (0,\bar{\lambda}_n) \supset (0,\bar{\lambda}_{n-1})$. Therefore $u(\lambda) < u_n(\lambda) < u_{n-1}(\lambda)$ for $\lambda \in (0,\bar{\lambda}_n)$ from Lemma 6.

Theorem 3: Let $\{\bar{\lambda}_n\}$ be as in Lemma 9; then $\bar{\lambda}_n \downarrow \lambda^*$.

Remark: For a concave f, $\lambda_n \uparrow \lambda^*$.

Proof: From Lemma 9(i), $\{\bar{\lambda}_n\}$ is a decreasing sequence bounded below by λ^* and hence $\bar{\lambda}_n \downarrow \bar{\lambda}_0^* \geqslant \lambda^*$.

If $\bar{\lambda}_0^* > \lambda^*$ then $\bar{\lambda}_n \geqslant \lambda^* + 2\epsilon$ for all n and some $\epsilon > 0$. Consequently $\nu_n(\lambda)$ is defined on $(0,\lambda^* + 2\epsilon)$, from Lemma 9 (iii), and $\nu_n(\bar{\lambda}_n) < \nu_n(\lambda^* + \epsilon)$ there. Now $\{u_n(\lambda^* + \epsilon)\}$ is an increasing sequence, from Corollary 3 (i). If it is uniformly bounded then it must converge uniformly to some positive solution $\bar{u}(\lambda^* + \epsilon)$ of (2) as in Theorem 1. This implies that $\lambda^* + \epsilon \leqslant \lambda^*$. Hence $u_n(\lambda^* + \epsilon) \underset{n \to \infty}{\to} \infty$ at least for one $x_0 \in D$. Since $u_n(\lambda^* + \epsilon)$ is continuous on D and increasing, it can be made arbitrarily large, by increasing n, on a neighborhood D_0 of x_0. Positivity of $G_{f'(u_n)}(x;\xi)$ on $D \times D$ implies that $u_n(\lambda^* + \epsilon) \underset{n \to \infty}{\to}$ for each $x \in D$. Now from Lemma 7 it follows that $\nu_n(\lambda^* + \epsilon) \underset{n \to \infty}{\to} \bar{\mu}(\infty)$, which implies that $\nu_n(\bar{\lambda}_n) \underset{n \to \infty}{\to} \bar{\mu}(\infty) \leqslant \lambda^*$. This is a contradiction since $\bar{\lambda}_n > \lambda^*$. Hence $\bar{\lambda}_0^* = \lambda^*$.

4. CONCLUDING REMARKS

The approximations $\lambda_n, \bar{\lambda}_n$ to λ^* of Sec. 3 are the fixed points of decreasing functions $\mu_n(\lambda)$, $\nu_n(\lambda)$ of λ on some set containing properly the intervals $(0,\lambda_n]$, $(0,\bar{\lambda}_n]$, respectively. Consider the case of λ_n. If $\lambda \neq \lambda_n$ then either $\mu_n(\lambda) > \lambda_n > \lambda$ or $\mu_n(\lambda) < \lambda_n < \lambda$. Therefore $\lambda_{n0} = \min[\lambda,\mu_n(\lambda)] \leqslant \lambda_n \leqslant \max[\lambda,\mu_n(\lambda)] = \lambda_{n1}$ for any λ. Pick some $\epsilon < 1$ and let

$$\begin{aligned} a_m &= (1-\epsilon)\lambda_{n(2m)} + \epsilon\lambda_{n(2m+1)}, \lambda_{n(2m+2)} \\ &= \max[\lambda_{n(2m)}, \min\{a_m, \mu_n(a_m)\}], \lambda_{n(2m+3)} \\ &= \min[\lambda_{n(2m+1)}, \max\{a_m, \mu_n(a_m)\}], \text{ for } m = 0,1,2,\cdots. \end{aligned}$$

It is easy to see that $\lambda_{n(2m+1)} \downarrow \lambda_n \uparrow \lambda_{n(2m)}$. The same method with obvious change of symbols is applicable in approximating $\bar{\lambda}_n$ except for the following. The function $\nu_n(\lambda)$ is defined on $(0,\bar{\lambda}_{n-1})$ only. Therefore the initial value $\lambda < \bar{\lambda}_{n-1}$ to obtain $\bar{\lambda}_{n0}, \bar{\lambda}_{n1}$, must be close enough to $\bar{\lambda}_n$ to ensure that $a_0 < \bar{\lambda}_{n-1}$ in order to guarantee the existence of the approximating sequences. However, this poses no serious problem as for $n = 0, \bar{\lambda}_0 = \nu_0(0) = \nu_0(\lambda)$ and hence for $n = 1$ any $\lambda < \bar{\lambda}_0$ will serve the purpose. Further, if $\bar{\lambda}_n$ has been approximated well from below, such a bound will be a suitable λ for $\bar{\lambda}_{n+1}$. Thus suitable starting values are straightforward to find.

For a concave f, to approximate λ^* by the present method is less satisfactory than the available ones. However, if this method is to be used then it is easy to check that the iterative method enables one to approximate $\lambda_n, \bar{\lambda}_n$ from below. To be precise, let $\lambda_{n0} \leqslant \lambda^*$ and

$\lambda_{n(m+1)} = \mu_n(\lambda_{n(m)}), m = 0,1,2,\cdots$. Then $\lambda_{n(m)} \uparrow \lambda_n \uparrow \lambda^*$. This result holds also with $\bar{\lambda}_{n(m)}$ replacing $\lambda_{n(m)}$ for each m. In case of a convex f, the iterative method will produce lower and upper bounds which may not converge.[9] It is pertinent here that if $f'(\phi), f''(\phi)$, and $f'''(\phi)$ exist and are positive for for $\phi > 0$ then the iterative method to determine the fixed point λ_n of $[\lambda + (1 - \lambda/\mu_n(\lambda))/\delta_n(\lambda)] > \lambda_n$ where $\delta_n(\lambda) = d(\lambda/\mu_n(\lambda))/d\lambda$ will produce converging upper bounds $\hat{\lambda}_{nm}$. The lower bounds then clearly are given by $\mu_n(\hat{\lambda}_{nm})$. This result holds also by replacing $\mu_n(\lambda)$ by $\nu_n(\lambda)$ and λ_n by $\bar{\lambda}_n$. Here again, as above, the initial value should be close to $\bar{\lambda}_n$ which is available from an approximation to $\bar{\lambda}_{n-1}$. The proof of the above result, although straightforward, is rather lengthy. Also it is of a limited value and computationally less convenient than the min-max method. Therefore a proof is omitted.

ACKNOWLEDGMENT

This work was supported by the National Sciences and Engineering Research Council of Canada under Grant No. A 3604 (to H. O. Pritchard).

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Inequalities in isotropic homogeneous turbulence theory

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(Received 13 May 1981; accepted for publication 28 August 1981)

It is postulated that the energy spectrum function is the Laplace transform of a nonnegative distribution ϕ. The principal physical parameters in the longitudinal correlation function are then expressed in terms of ϕ integrals and interrelated by Hölder inequalities, to yield experimentally confirmed results like $L_p \geqslant 1.825\lambda$.

PACS numbers: 47.25.Cg, 47.10. + g

Determined in theoretical detail by Navier–Stokes transfer and dissipation of energy,[1–3] the longitudinal correlation function $f(r,t)$ manifests certain general analytic properties for all types of isotropic homogeneous turbulence. It is given generically for small $r \lesssim \lambda\,(t) \equiv (15\nu u^2/\epsilon)^{1/2}$ by the alternating power series

$$f = 1 - \frac{r^2}{2\lambda^2} + \frac{5(B+1)}{56}\frac{r^4}{\lambda^4} - O\left(\frac{r^6}{\lambda^6}\right), \quad 0 < r \lesssim \lambda \tag{1}$$

in which B is the dimensionless "broadness" parameter.[4] For large r it has the asymptotic form[5–8]

$$f = Ir^{-3} - Jr^{-4} + O(L_p^5/r^5), \quad r \gtrsim 3L_p \tag{2}$$

in which $I(t) \equiv \lim_{r\to\infty}(r^3 f)$, $J(t) \equiv \lim_{r\to\infty} r^4(3f + r\partial f/\partial r)$, and $L_p(t) \equiv \int_0^\infty f\,dr$ are positive quantities. Moreover, an especially simple and universal r dependence is associated with grid-generated strong turbulence during the initial period (grid Reynolds numbers UM/ν from 12800 to 81000 and $u\lambda/\nu \gtrsim 40$) where experiments[9] show that f is independent of t for $r \gtrsim \lambda$ and given by the empirical relation[8]

$$f = [1 + (0.770)(r/M)]^{-3}, \quad r \gtrsim \lambda\,(\sim 0.1M) \tag{3}$$

from which the quantities in (3) are obtained as

$$I = 2.19M^3, \quad J = 8.54M^4 \quad \text{with} \quad L_p = 0.649M. \tag{4}$$

The purpose of this paper is to point out that stringent inequality relations obtain for the physical parameters λ, B, I, J, and L_p in (1) and (2) if the energy spectrum function is expressible as the Laplace transform of a nonnegative distribution:

$$E(\kappa,t) = \tfrac{1}{4}u^2\kappa^2 \int_0^\infty \phi(s,t)\,e^{-\kappa s}\,ds, \quad \phi \geqslant 0. \tag{5}$$

Such a representation is guaranteed by the Post–Widder[10,11] real inversion formula

$$\phi(s,t) = \tfrac{1}{3}u^{-2} \lim_{n\to\infty}\left\{\frac{(-1)^n\kappa^{n+1}}{n!}\frac{\partial^n}{\partial\kappa^n}[\kappa^{-2}E(\kappa,t)]\right\}_{\kappa = n/s} \tag{6}$$

if $(-1)^n\partial^n[\kappa^{-2}E(\kappa,t)]/\partial\kappa^n$ is nonnegative for all κ with n sufficiently large; moreover, the approximate real inversion formulas[12] based on (6) yield patently nonnegative ϕ for the energy spectra of practical interest. The normalization condition that follows from (5),

$$\int_0^\infty s^{-3}\phi(s,t)\,ds = \tfrac{1}{3}u^{-2}\int_0^\infty E(\kappa,t)\,d\kappa = 1, \tag{7}$$

shows that ϕ must vanish strongly for small s. This will indeed be the case if the analytic continuation $f(z,t)$ for complex $z = r + is$ is regular in the first quadrant ($r > 0$, $s > 0$), as seen by converting the Fourier transform[13] into a Laplace transform:

$$E(\kappa,t) = \frac{u^2}{\pi}\left(\kappa^2\frac{\partial^2}{\partial\kappa^2} - \kappa\frac{\partial}{\partial\kappa}\right)F(\kappa,t), \tag{8}$$

$$F(\kappa,t) \equiv \int_0^\infty f(r,t)(\cos\kappa r)\,dr = \mathrm{Re}\int_0^\infty f(r,t)e^{i\kappa r}\,dr$$
$$= \mathrm{Re}\int_0^\infty f(is,t)e^{-\kappa s}i\,ds = -\int_0^\infty [\mathrm{Im}\,f(is,t)]e^{-\kappa s}\,ds. \tag{9}$$

In (9), the integration path has been rotated through the first quadrant from the physical positive real axis to the positive imaginary axis, a change effected by the replacement $r \to is$. It is tacitly understood that $f(is,t) \equiv \lim_{r\to 0+} f(is + r, t)$ in the final member of (9), with the limit taken after integration in the event that $f(z,t)$ has a singularity on the positive imaginary axis [see, e.g., (25) below]. Notice that in the case of (1) and (3),

$$\mathrm{Im}\,f(is,t) = \begin{cases} 0 & \text{for } 0 < s \lesssim \lambda, \\ \dfrac{s^3 - 3s}{(1+s^2)^3} & \text{for } s \gtrsim \lambda, \end{cases} \tag{10}$$

in a convenient system of length units such that $M = (0.770)$; more generally, from (1) and (2),

$$\mathrm{Im}\,f(is,t) = \begin{cases} 0 & \text{for } 0 < s \lesssim \lambda, \\ Is^{-3} - O(L_p^5/s^5) & \text{for } s \gtrsim 3L_p, \end{cases} \tag{11}$$

with $\mathrm{Im}\,f(is,t)$ negative over an s interval above λ before turning postive for larger s. Substituting (9) into (8) and performing an integration by parts after the κ differentiations, one obtains (5) with

$$\phi(s,t) = \frac{4}{3\pi}\left[\int_s^\infty \mathrm{Im}\,f(is',t)s'\,ds' - s^2\mathrm{Im}\,f(is,t)\right]. \tag{12}$$

Since

$$\int_0^\infty \mathrm{Im}\,f(is',t)s'\,ds' = -\,\mathrm{Im}\int_0^\infty f(r,t)r\,dr = 0, \tag{13}$$

it follows from (11) and (12) that $\phi(s,t) = 0$ for $0 < s \lesssim \lambda$.

The useful representation for f itself emerges by putting (5) into the energy spectrum Fourier transform[13] and carrying out the integration over κ:

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$$f(r,t) = 2u^{-2}\left(r^{-3} - r^{-2}\frac{\partial}{\partial r}\right)\int_0^\infty E(\kappa,t)\kappa^{-3}(\sin\kappa r)\,d\kappa$$
$$= \tfrac{3}{2}r^{-3}\int_0^\infty \left[\left(\tan^{-1}\frac{r}{s}\right) - rs(r^2+s^2)^{-1}\right]\phi(s,t)\,ds$$
$$= \int_0^\infty \left[1 - \frac{6}{5}\left(\frac{r}{s}\right)^2 + \frac{9}{7}\left(\frac{r}{s}\right)^4 - \cdots\right]s^{-3}\phi\,ds$$
$$= \tfrac{3}{2}r^{-3}\int_0^\infty \left[\frac{\pi}{2} - 2sr^{-1} + \cdots\right]\phi\,ds. \tag{14}$$

From (14) one obtains ϕ-integral formulas for the coefficients in (1) and (2), namely

$$\lambda^{-2} = \frac{12}{5}\int_0^\infty s^{-5}\phi\,ds, \tag{15}$$

$$B+1 = \frac{5}{2}\int_0^\infty s^{-7}\phi\,ds\left(\int_0^\infty s^{-5}\phi\,ds\right)^{-2}, \tag{16}$$

$$I = \frac{3\pi}{4}\int_0^\infty \phi\,ds, \tag{17}$$

$$J = 3\int_0^\infty s\phi\,ds, \tag{18}$$

as well as

$$L_p = \frac{3\pi}{8}\int_0^\infty s^{-2}\phi\,ds \tag{19}$$

by direct integration over r of the third member of (14). Notice that the Schwarz inequality and normalization condition (7) imply $B \geqslant \frac{1}{2}$ according to (16), with equality only for the academic Birkhoff form (Ref. 6, p. 34), for which $\phi(s,t) = a^3\delta(s-a)$ with $a = a(t) > 0$. Indeed, the experimentally observed broadness values[4] are all greater than $\frac{1}{2}$. The Hölder inequality

$$\int_0^\infty \phi\,ds \leqslant \left(\int_0^\infty s\phi\,ds\right)^{3/4}\left(\int_0^\infty s^{-3}\phi\,ds\right)^{1/4} \tag{20}$$

in combination with (7), (17), and (18) yields

$$J \geqslant (0.957)I^{4/3}. \tag{21}$$

Similarly, obvious Hölder inequalities applied to (7), (17), (18), and (19) produce

$$(1.441)L_p^{\,3} \leqslant I \leqslant (1.073)J^{2/3}L_p^{\,1/3}. \tag{22}$$

Finally, the Hölder inequality

$$\int_0^\infty s^{-3}\phi\,ds \leqslant \left(\int_0^\infty s^{-5}\phi\,ds\right)^{1/3}\left(\int_0^\infty s^{-2}\phi\,ds\right)^{2/3} \tag{23}$$

in combination with (7), (15), and (19) yields the remarkable relation between the basic scale parameters

$$L_p \geqslant (1.825)\lambda. \tag{24}$$

Other inequalities involving the parameters (15)–(19) are also obtainable in this manner.

The values in (4) for grid-generated strong turbulence are clearly consistent with the general inequalities (21), (22), and (24), for λ is less than $0.2M$ in these initial period experiments. A very stringent test of the inequalities is provided by the experimental measurements[14] on grid-generated weak turbulence ($UM/\nu < 10^3$, $u\lambda/\nu \lesssim 30$). Since this weak turbulence features[4] $B = 1.80$, the longitudinal correlation function is not substantially dissimilar from Birkhoff's $B = 1.50$ academic case, for which (21), (22), and (24) all hold as exact equalities. From the weak turbulence empirical relation[14,15] (see Table I)

TABLE I. Comparison of experimental f values for the grid-generated weak turbulence (Ref. 14, Fig. 9 and Ref. 15) with values given by Eq. (25).

r/λ	0	1	2	3	4	5	6	7
f	1	0.68	0.33	0.18	0.12	0.07	0.05	0.03
f[Eq. (25)]	1	0.667	0.333	0.182	0.111	0.069	0.048	0.034

$$f = \begin{cases} (1 + r^2/2\lambda^2)^{-1} & \text{for } r < 5\lambda \\ 19(\lambda/r)^3 - 52(\lambda/r)^4 & \text{for } r \geqslant 5\lambda \end{cases} \tag{25}$$

it follows that

$$I = 19\lambda^3, \quad J = 52\lambda^4, \quad L_p = (2.06)\lambda. \tag{26}$$

The weak turbulence parameter values in (26) are indeed also consistent with the general inequalities (21), (22), and (24).

A final check on the correctness of the inequalities is afforded by experimental data[16] on waterfall-generated turbulence at very high intrinsic Reynolds numbers $u\lambda/\nu \gtrsim 10^3$. From the measured value[16] $L_p = 27.5\lambda$ and the empirical relation (see Table II)

$$f \cong 9.00\times 10^4(\lambda/r)^3 - 4.74\times 10^6(\lambda/r)^4 \quad \text{for } r \gtrsim 80\lambda \tag{27}$$

it follows that

$$I = 9.00\times 10^4\lambda^3, \quad J = 4.74\times 10^6\lambda^4, \tag{28}$$

and it is readily verified that (21) and (22) are again satisfied by the latter values.

Hence, the inequalities are confirmed by experiment. In terms of the longitudinal correlation function the main results (21) and (24) take the form

$$\lim_{r\to\infty}\left[f^{-4/3}\left(3f + r\frac{\partial f}{\partial r}\right)\right] \geqslant 0.957, \tag{29}$$

$$\int_0^\infty f(\lambda\alpha,t)\,d\alpha \geqslant 1.825. \tag{30}$$

It is interesting to note that the empirical forms (3), (25), and (27) have the common property $\partial f/\partial t \geqslant 0$ for all r and $t \geqslant 0$ because λ is monotone increasing with increasing t.[4] This implies that the right side of the Kármán–Howarth equation[17,13]

$$\frac{\partial f}{\partial t} = 2\nu\left(\frac{\partial^2 f}{\partial r^2} + \frac{4}{r}\frac{\partial f}{\partial r}\right) - u^{-2}\frac{du^2}{dt}f + u^{-2}K \tag{31}$$

is likewise nonnegative for all r and $t \geqslant 0$. Defined implicitly by the formula

$$\langle u_j(\mathbf{x},t)u_k(\mathbf{x},t)u_k(\mathbf{x}+\mathbf{r},t)\rangle \equiv \tfrac{1}{2}r_jK(r,t), \tag{32}$$

$K = K(r,t)$ on the right side of (31) is concomitant with the

TABLE II. Comparison of experimental f values for the waterfall-generated strong turbulence (Ref. 16, Fig. 2) with values given by Eq. (27).

r^*	140	150	160	170	180
$r/\lambda = r^*/1.74$	80.5	86.2	92.0	97.7	103.4
f	0.060	0.055	0.050	0.045	0.040
f[Eq. (27)]	0.0597	0.0547	0.0494	0.0445	0.0399

inertial transfer of energy.[1-3] If one introduces a representation for K similar to (14),

$$K(r,t) \equiv \tfrac{1}{2}u^2 r^{-3} \int_0^\infty \left[\tan^{-1} \frac{r}{s} - rs(r^2+s^2)^{-1} \right] \psi(s,t)\, ds, \tag{33}$$

and substitutes (14) and (33) into (31), one obtains an adjoint dynamical equation for nonnegative $\phi(s,t)$,

$$\frac{\partial \phi}{\partial t} = -2\nu \frac{\partial^2 \phi}{\partial s^2} - u^{-2} \frac{du^2}{dt} \phi + \psi, \tag{34}$$

where the viscous "antidiffusion" term emerges after performing two integrations by parts with respect to s; this viscous term on the right side of (34) is strictly one dimensional, in contrast to the radial diffusion terms in (31). To guarantee $\phi(s,t) \geqslant 0$ for all s and $t \geqslant 0$ in the context of a Phragmén–Lindelöf maximum principle,[18,19] one must put a suitable inequality condition on ψ in (34).

ACKNOWLEDGMENT

This work was supported by NASA grant NAG1-110.

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Dynamic polarizability of the double quadratic and multiquadratic chains with anharmonic coupling

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(Received 22 May 1981; accepted for publication 26 June 1981)

We study the dynamic polarizability of a linear chain of atoms interconnected by springs and subjected to a double quadratic (D-Q) or multiquadratic (M-Q) substrate potential in the presence of a weak nonlinear coupling term between adjacent particles. The results obtained by Trullinger on the D-Q model with linear coupling are reviewed and the same formalism is extended to calculate the modified kink waveform in the presence of nonlinear coupling and the dynamic polarizability of this modified kink. The simplicity of the model allows us to carry out analytically all the calculations. We show that the presence of kinks in such an anharmonic chain enhances the effect of coupling nonlinearities.

PACS numbers: 63.10. + a, 03.40.kf

I. INTRODUCTION

The model of a linear chain of atoms interconnected by springs and subjected to a periodic substrate potential is currently widely studied both because of its intrinsic mathematical interest and because of the large number of physical situations for which this model represents the simplest formulation which includes the essence of the process. Two kinds of substrate potential are generally considered: a double well potential whose prototype is the ϕ^4 potential and a periodic potential like the sinusoidal potential of the Sine–Gordon (S-G) chain. In the continuum limit these two models give rise to nonlinear wave equations which admit large-amplitude solitary waves or soliton solutions that retain their shape during propagation. The ϕ^4 model has recently received a great deal of attention[1–5] as a model of domain walls in displacive phase transitions, while the areas of applications of the S-G model include dislocation lines in imperfect crystals,[6] ion motions in some superionic conductors,[7–9] and charge density waves in metals.[10–12] Statistical mechanics investigations[1,2,4,13] have shown that solitons behave as elementary excitations at finite temperature and phenomenologies which treat them as an ideal gas of particles have been developed.[1,2,13] In addition the influence of various types of perturbing forces on solitons has been investigated.[14] A topic of particular importance in the context of domain wall in ferroelectrics is the manner in which kinks respond to an oscillating electric field, that is to say, the calculation of the generalized susceptibility[15] of the chain in the presence of solitons. This topic is also related to the dielectric or FIR response of imperfect crystals (for instance crystals with dislocations) or crystalline solids (like superionic conductors) in which the correlation length of large-amplitude atomic motions is expected to be sufficient to allow the formation of collective modes randomly moving across the crystal.[7–9] In this context the double-well model describes localized motions (like molecular rotations in some molecular crystals)[16,17] and the periodic potential describes diffusive motions (like ionic diffusion in fast-ions conductors).[7–9] Moreover in this case, since large atomic displacements which are no longer negligible with respect to the unit cell dimensions are involved, it is of great physical interest to introduce in the model nonlinear coupling terms between adjacent particles to take into account the anharmonicity of pair potentials in solids. It is the aim of this paper to investigate the dynamic polarizability of a linear chain bearing solitons when a small cubic nonlinearity is introduced in the spring connecting adjacent particles in the double well or periodic potential models.

The response of a ϕ^4 kink to an oscillating field has been studied recently by Theodorakopoulos *et al.*[5] and Lee and Trullinger[5] have investigated the generalized susceptibility of kink solutions of the nonlinear Klein Gordon equation and applied their formalism to the S–G and ϕ^4 kinks. Allroth and Mikeska[18] calculated the dynamical structure factor of the S–G chain. But, even for the special case of homogeneous applied fields the dynamic polarizability of the ϕ^4 or S–G kinks are extremely cumbersome to evaluate[15] and require the performance of infinite summations. Consequently the extension of these calculations to S–G and ϕ^4 systems in the presence of nonlinear coupling terms appears to be very difficult. So we investigate alternate models which preserve the essential features of the ϕ^4 or S–G model but which lead to much simpler calculations.[15,19] A double-quadratic (D-Q) potential[15] is used for the double-well model instead of the ϕ^4. This potential consists of two displaced parabolas [Fig. 1(a)] and gives rise to solitary wave solutions of the unperturbed equation of motion. In a similar manner the sinusoidal substrate potential is replaced by an array of parabolas[19] [Fig. 1(b)] henceforth referred to as the multiquadratic potential (M-Q). These two models are more tractable analytically than the ϕ^4 or S–G models since they give rise to wave equations which are piecewise linear in the case of linear coupling, allowing us to perform analytically the computation in the presence of nonlinear coupling in the framework of a perturbation theory. The dynamic polarizability of the D-Q chain with linear coupling in the presence of a static kink was first studied by Trullinger[15] and our investigations use the same formalism, especially the expansion technique proposed by Fogel *et al.*[14,20] which makes use of the completeness property of small oscillations about the kink waveform.

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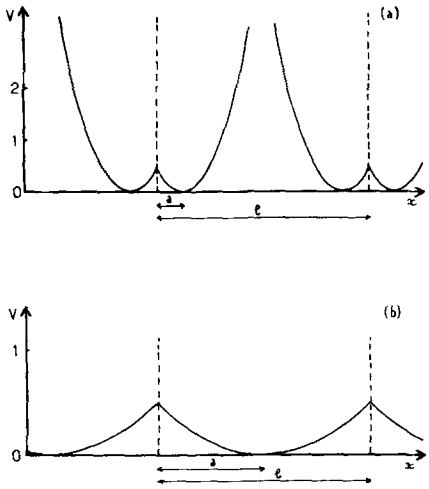

FIG. 1. Substrate potential of the double quadratic (D-Q) (a) and multiquadratic (M-Q) (b) chains.

The plan of this paper is as follows. In Sec. II we describe the D-Q and M-Q models. The results obtained by Trullinger[15] on the D-Q chain with linear coupling in the presence of a static kink are summarized and extended to the M-Q model. The results are compared with those of the ϕ^4 or S–G models. In Sec. III the nonlinear coupling term is introduced and the new soliton solutions are obtained. The generalized susceptibility of the D-Q or M-Q chain with nonlinear coupling is then computed in Sec. IV. We find that kinks enhance the effects of the nonlinear coupling terms; in their presence the nonlinear coupling contribution to the generalized susceptibility appears in the first-order term of the perturbation expansion rather than in the second-order term. In Sec. V we give a brief summary.

II. THE D-Q AND M-Q MODELS WITH HARMONIC COUPLING

In this section we describe the models studied and summarize the method used by Trullinger[15] to compute the generalized susceptibility of a static kink in the D-Q model with harmonically-coupled particles since it constitutes our starting point for further calculations. We then compare the results with results previously published on the ϕ^4 or S–G models and we show that the dependence of the main features of the susceptibility on the specific form of the potential is rather small.

The systems under consideration [Figs. 1(a) and 1(b)] consist of one-dimensional chains of harmonically-coupled oscillators governed by the following Hamiltonian:

$$H = \sum_n \tfrac{1}{2}m\dot{u}_n^2 + \tfrac{1}{2}K_0(u_{n+1} - u_n)^2 + V_0(u_n), \tag{2.1}$$

where u_n is the displacement coordinate of the nth oscillator. The first term represents the kinetic energy carried by the displacement field (a dot denotes a time derivative) and the second term is the strain energy arising from the harmonic coupling (coupling constant K_0) between displacements at neighboring lattice sites.

The potential energy term has different expressions for the D-Q or M-Q models:

$$V_0^{DQ}(u) = \tfrac{1}{2}m\omega_0^2(|u| - a)^2,$$

$$V_0^{MQ}(u) = \begin{cases} \tfrac{1}{2}m\omega_0^2(u-a)^2, & \text{for } 0 \leqslant u \leqslant 2a, \\ V_0^{MQ}(u - 2na), & \text{for } u < 0 \text{ or } u > 2a \end{cases}$$

(in the last expression the value of n is chosen so that $0 \leqslant u - 2na \leqslant 2a$). The constant ω_0 represents the limiting frequency of long wavelength phonons. The spacing between adjacent wells is designed by a and l denotes the length of the unit cell in the chain. For the D-Q chain $l > 2a$ while for the M-Q model $l = 2a$ (Fig. 1). Introducing the dimensionless displacement coordinate $\phi_n = u_n/a$, the Hamiltonian (2.1) is written

$$H = Al\sum_n \tfrac{1}{2}\dot{\phi}_n^2 + \tfrac{1}{2}\frac{C_0^2}{l^2}(\phi_{n+1} - \phi_n)^2 + \omega_0^2 V(\phi_n). \tag{2.2}$$

The constant $A = ma^2/l$ sets the energy scale and $C_0^2 = K_0 l^2/m$ is the limiting velocity of the kink.

The dimensionless potential function is

$$V^{DQ}(\phi) = \tfrac{1}{2}(|\phi| - 1)^2 \text{ for the D-Q model,}$$

and

$$V^{MQ}(\phi) = \begin{cases} \tfrac{1}{2}(\phi - 1)^2, & \text{for } 0 \leqslant \phi \leqslant 2, \\ V^{MQ}(\phi - 2n), & \text{for } 0 \leqslant \phi - 2n \leqslant 2, \end{cases}$$

for the M-Q model.

It is important to notice that for $-2 < \phi < 2$,

$$V^{DQ}(\phi) = V^{MQ}(\phi) = \tfrac{1}{2}(|\phi| - 1)^2. \tag{2.3}$$

We restrict ourselves to the continuum approximation, i.e., we assume that the coupling between neighboring sites is strong enough to ensure that variations of ϕ from site to site are quite small. The relevant length scale is $d = C_0/\omega_0$ and we assume that $d \gg l$. In this limit, kinks become well-defined excitations[21,22] with long lifetimes and the Hamiltonian (2.2) is replaced by

$$H = A\int dx \left\{ \tfrac{1}{2}[\dot{\phi}(x,t)]^2 + \tfrac{1}{2}C_0^2[\phi_x(x,t)]^2 + \omega_0^2 V(\phi) \right\}, \tag{2.4}$$

where $\phi_x(x,t) = (\partial/\partial x)\phi(x,t)$ is the continuum limit of $(\phi_{n+1} - \phi_n)/l$.

The Hamiltonian equation following from Eq. (2.4) is

$$\ddot{\phi} - C_0^2\phi_{xx} + \omega_0^2\frac{\partial V}{\partial \phi} = 0. \tag{2.5}$$

We are concerned only with linear "phonon" solutions and with kink or antikink solutions. The linear solutions are oscillations around the equilibrium positions $\phi_e = \pm 1$ whose magnitude must be less than 1 ($|\phi - \phi_e| < 1$) but is not required to be infinitesimally small since the individual potential wells are perfectly harmonic for $|\phi - \phi_e| < 1$. For the kink solution we impose the conditions $\phi(+\infty) = 1$ and $\phi(-\infty) = -1$ and for antikink solutions the sign of ϕ is reversed. In the case of the M-Q potential additional multikink solutions may exist with limiting values $\phi(\pm\infty) = \pm n$ but they require much more energy to be created and they are neglected here. With this restriction, the values of ϕ are confined to the -2, $+2$ range so that $V(\phi)$ has the same expression $V(\phi) = \frac{1}{2}(|\phi| - 1)^2$ for the two models. The motions in real space are different, but in the

dimensionless variables the results are identical for the two models. Of course this would no longer be true if multikink solutions were involved or if statistical mechanics studies were performed.[13] Configurations involving several kinks are essentially different for the two models, since only an antikink can follow a kink in the D-Q model while kinks or antikinks do not necessary alternate in the M-Q model. But, as mentioned in the following, the dynamical polarizabilities of kinks or antikinks are identical so that, for our purpose, the two models give identical results when they are expressed in dimensionless variables and this is an interesting feature of these models.

Consequently Eq. (2.5) yields

$$\ddot{\phi} - C_0^2\phi_{xx} + \omega_0^2(|\phi| - 1)\mathrm{sgn}(\phi) = 0 \tag{2.6}$$

for the D-Q and M-Q models. This equation has been solved by Trullinger[15] and we first summarize his results. The linear "phonon" solutions have the form

$$\phi_k \pm 1 = \phi_0 \cos(kx - \omega_k t) \quad (|\phi_0| < 1) \tag{2.7}$$

with the dispersion relation

$$\omega_k^2 = \omega_0^2 + C_0^2 k^2. \tag{2.8}$$

The travelling kink solutions are

$$\phi_S^{(v)} = \pm \mathrm{sgn}\left[\frac{x - vt}{(1 - v^2/C_0^2)^{1/2}}\right] \times\left[1 - \exp\left(-\frac{|x - vt|}{d(1 - v^2/C_0^2)^{1/2}}\right)\right], \tag{2.9}$$

where $+(-)$ is appropriate to the kink (antikink) solution and v is the velocity of the kink. The small oscillations in the presence of a kink at rest at the origin ($x = 0$) are computed since they form a complete orthonormal set of functions which may be used to expand deviations of the kink waveform in the presence of external perturbations. $\phi(x,t)$ is written

$$\phi(x,t) = \phi_S^{(0)} + \Psi(x,t),$$

where $\phi_S^{(0)}$ is the static kink waveform deduced from Eq. (2.9). The small deviation $\Psi(x,t)$ is governed by

$$\ddot{\Psi}(x,t) - C_0^2\Psi_{xx}(x,t) + \omega_0^2\Psi(x,t)\{1 - 2d\delta(x)\} = 0,$$

where $\delta(x)$ is the Dirac delta function.

Assuming solutions of the form

$$\Psi(x,t) = f(x)e^{-i\omega t}$$

and introducing the dimensionless quantities

$$z = x/d, \quad \tau = \omega_0 t, \quad K = kd, \quad \bar{\omega}_K = \omega_k/\omega_0,$$

the following expressions are obtained for the functions $f(z)$:

$$f_b(z) = \exp(-|z|), \tag{2.10a}$$

$$f_{K_-}(z) = \frac{1}{\sqrt{\pi}}\sin K_- z \quad (K_- < 0), \tag{2.10b}$$

$$f_{K_+}(z) = \frac{1}{\sqrt{\pi}(1 + K_+^2)^{1/2}} \times [K_+ \cos K_+ z - \sin K_+ |z|] \quad (K_+ > 0). \tag{2.10c}$$

Note that in terms of the dimensionless variables the limiting velocity of kinks is $\bar{c}_0 = 1$. The "bound state" solution $f_b(z)$ corresponds to the translation mode of the kink. The "continuum" states $f_{K\pm}$ are classified by their parity under reflection through $x = 0$ and the corresponding eigenvalues $\bar{\omega}_K$ are given by the dispersion relation (2.8).

Once this set of functions is obtained they are used to compute the linear response of a kink at rest at the origin to an external applied field $E(z,\tau)$ which couples linearly to the displacement field. Equation (2.6) now assumes the dimensionless form

$$\frac{\partial^2\phi}{\partial\tau^2} - \frac{\partial^2\phi}{\partial z^2} + (|\phi| - 1)\mathrm{sgn}(\phi) + \Gamma\frac{\partial\phi}{\partial\tau} = E(z,\tau). \tag{2.11}$$

Γ is a dimensionless damping constant and the damping term $\Gamma\partial\phi/\partial\tau$ is introduced to ensure that the response of the system remains small if $E(z,\tau)$ is small in magnitude so that Eq. (2.11) may be solved in the framework of linear response theory (we assume that $E(z,\tau)$ does not contain a term which is constant in time). Assuming solutions of the form

$$\phi(z,\tau) = \phi_s^{(0)}(z) + \Delta\phi(z,\tau),$$

linearization of Eq. (2.11) in $\Delta\phi$ gives

$$\frac{\partial^2\Delta\phi}{\partial\tau^2} - \frac{\partial^2\Delta\phi}{\partial z^2} + (1 - 2\delta(z))\Delta\phi + \Gamma\frac{\partial\Delta\phi}{\partial\tau} = E(z,\tau). \tag{2.12}$$

Note that $\phi_s^{(0)}(z)$ may be either a kink or an antikink; Eq. (2.12) is not modified and this shows that the responses in the presence of a kink or an antikink are identical. From the point of view of phonons an antikink is indistinguishable from a kink.[23] The linear equation (2.12) is solved by a time Fourier transformation and expansion in terms of the complete set $\{f_b(z), f_{K_+}(z), f_{K_-}(z)\}$. $\Delta\phi$ is expressed in the form

$$\Delta\phi(z,\tau) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\Omega\, e^{i\Omega\tau}\Delta\hat{\phi}(z,\Omega) = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\Omega\, e^{i\Omega\tau}\int_m \Delta\hat{\phi}_m(\Omega) f_m(z), \tag{2.13}$$

where the generalized summation symbol $\int_m$ denotes the following

$$\int_m f_m = f_b + \int_{-\infty}^{0} dK_- f_{K_-} + \int_0^{\infty} dK_+ f_{K_+}.$$

The coefficients $\Delta\hat{\phi}_m(\Omega)$ of the expansion of $\Delta\hat{\phi}(z,\Omega)$ are given by

$$\Delta\hat{\phi}_m(\Omega) = \hat{E}_m(\Omega)/[\bar{\omega}_m^2 - \Omega^2 + i\Gamma\Omega], \tag{2.14}$$

where $\hat{E}_m(\Omega)$ denotes the coefficients of the expansion of the time Fourier transform $\hat{E}(z,\Omega)$ of $E(z,\tau)$ in terms of the same basis. The response function $\alpha(z,z';\Omega)$ defined by

$$\Delta\hat{\phi}(z,\Omega) = \int_{-\infty}^{\infty} dz'\,\alpha(z,z';\Omega)\hat{E}(z',\Omega) \tag{2.15}$$

is expressed in terms of $\{f_j\}$

$$\alpha(z,z';\Omega) = \int_j \frac{f_j(z)f_j(z')}{\bar{\omega}_j^2 - \Omega^2 + i\Gamma\Omega}. \tag{2.16}$$

As we consider only that part of the response corresponding to the deformation of the kink waveform, the term $m = b$ is dropped from the j sum in Eq. (2.16). Making use of Eq.

(2.10b) and (2.10c) and performing the K integrations this becomes

$$\alpha(z,z';\Omega) = -\frac{i}{4Q}e^{iQ|z+z'|} + \frac{i}{4Q}e^{iQ|z-z'|} + \frac{i}{4Q}\frac{Q+i}{Q-i}e^{iQ(|z|+|z'|)} + \frac{i}{4Q}e^{iQ||z|-|z'||} + \frac{1}{1+Q^2}e^{-(|z|+|z'|)}, \quad (2.17)$$

where Q denotes the branch of $(\Omega^2 - 1 - i\Gamma\Omega)^{1/2}$ having a positive imaginary part. The response function $\alpha(z,z';\Omega)$ contains a term which measures the response of the displacement field far from the kink and another component which is the intrinsic response of the kink.

The generalized susceptibility is the Fourier transform of the response function[15]

$$\chi^{(0)}(p,q;\Omega) = \int_{-\infty}^{+\infty} dz \times \int_{-\infty}^{+\infty} dz'\, e^{-ipz}\, e^{-iqz'}\alpha(z,z';\Omega). \quad (2.18)$$

Substitution of Eq. (2.17) into (2.18) yields the result

$$\chi^{(0)}(p,q;\Omega) = \frac{2\pi}{q^2-Q^2}\delta(p+q) + \frac{2Q(Q+i)}{(Q^2-p^2)(Q^2-q^2)(Q^2+1)} + \frac{4}{(1+p^2)(1+q^2)(1+Q^2)}. \quad (2.19)$$

The first term is the phonons term and, recalling the definition of Q, one recognizes the usual Lorentzian shape. The last two terms arise from the presence of the kink and thus constitute the intrinsic susceptibility of the static kink as obtained by Trullinger.[15]

Trullinger[15] pointed out that the static kink contribution to the susceptibility is similar to that of a harmonic oscillator. However we call attention to the signs of the real and imaginary parts of the kinks' contribution to the susceptibility which are opposite to those of harmonic oscillators (or phonons). Thus kinks contribute to reduce the total response of the chain with respect to the total response of the kink-free system. This is associated with the reduction of allowed phonon states in the presence of kinks.[22] Moreover for the low values of the dimensionless damping ($\Gamma \lesssim 0.2$) two distinct contributions appear in the kinks' contribution to the susceptibility: in addition to the strong peak of the imaginary part mentioned by Trullinger[15] and arising from phonon backscattering, a smaller contribution corresponding to a diffuse absorption (positive contribution to the imaginary part) appears near the phonon peak ($\bar{\omega} = 1$). This diffuse absorption increases when Γ decreases and it is interesting to notice that, for low damping, the imaginary part of $\chi_s^{(0)}(p,q;\Omega)$ looks very similar to the qualitative absorption spectrum obtained by Theodorakopoulos in the limit of vanishing damping for the ϕ^4 model.[5] Since we have shown that our results in their dimensionless form also apply to the M-Q model, they can also be compared with the results previously published about the S–G chain. For this system Allroth and Mikeska[18] deduced a reduction of the small amplitude excitations (magnons in their case) density of states in the presence of solitons. Moreover they showed that the dynamical-structure factor in the limit of vanishing damping acquires a Lorentzian line shape characterized by a width which is roughly proportional to the kink density. This last result is in agreement with our computations, which show that the half-width of the susceptibility imaginary part increases in the presence of kinks. However this effect is less pronounced for the D-Q or M-Q models than for the S-G model. In spite of minor differences we observe that the main features of the response to an external applied field are similar for the D-Q (M-Q) and ϕ^4 (S–G) models. Although the D-Q and M-Q potentials are nonreflectionless for the phonons while the ϕ^4 or S–G are reflectionless we conclude that the effect of the specific form of the substrate potential on the generalized susceptibility is rather weak.

III. KINKS IN THE PRESENCE OF NONLINEAR COUPLING

In this section we introduce a cubic nonlinearity in the strain energy of the system associated with coupling between displacements at neighboring lattice sites and we derive a new form of the displacement field equation of motion. Then we solve this equation in the framework of a first-order perturbation theory to obtain a new kink waveform in the presence of nonlinear coupling. (In the following this kink will be referred to as the "modified kink.")

Introducing a cubic term in the strain energy, the Hamiltonian (2.1) is now written

$$H = \sum_n \left[\tfrac{1}{2}m\dot{u}_n^2 + \tfrac{1}{2}K_0(u_{n+1}-u_n)^2 + \tfrac{1}{6}\epsilon K_1(u_{n+1}-u_n)^3 + V_0(u_n)\right], \quad (3.1)$$

where the third term is the energy arising from the anharmonic coupling between adjacent particles (K_1 is a positive coupling constant). ϵ is a dimensionless constant which is used to specify the order of the perturbation calculation ($\epsilon \ll 1$). In terms of the dimensionless variables introduced in Sec. II, the Hamiltonian (3.1) is expressed in the form

$$H = Al\sum_n \tfrac{1}{2}\dot{\phi}_n^2 + \tfrac{1}{2}C_0^2 l^{-2}(\phi_{n+1}-\phi_n)^2 + \tfrac{1}{6}\epsilon k l^{-3}(\phi_{n+1}-\phi_n)^3 + \omega_0^2 V(\phi_n), \quad (3.2)$$

where $k = K_1 a l^3/m$ and the other terms have the same meaning as in Eq. (2.2). In the continuum limit the Hamiltonian (3.2) becomes

$$H = A\int dx \left[\tfrac{1}{2}\dot{\phi}^2 + \tfrac{1}{2}C_0^2\phi_x^2 + \tfrac{1}{6}\epsilon k\phi_x^3 + \omega_0^2 V(\phi)\right] \quad (3.3)$$

so that the Hamilton equation of motion of the displacement field is now

$$\ddot{\phi} - C_0^2\phi_{xx} - \epsilon k\phi_x\phi_{xx} + \omega_0^2\frac{\partial V}{\partial\phi} = 0 \quad (3.4)$$

instead of Eq. (2.5).

Since we still impose the conditions $\phi(+\infty) = 1(-1)$ and $\phi(-\infty) = -1(+1)$ for kinks (antikinks) solutions,

$\partial V/\partial\phi$ retains the same expression $(|\phi|-1)\,\mathrm{sgn}(\phi)$ for both D-Q and M-Q models so that Eq. (3.4) yields

$$\ddot{\phi} - C_0^2\phi_{xx} - \epsilon k\phi_x\phi_{xx} + \omega_0^2(|\phi|-1)\mathrm{sgn}(\phi) = 0. \quad (3.5)$$

Contrary to Eq. (2.6) the new equation of motion has no longer a covariant form; nevertheless it is still interesting to define the new variable $X = (x - vt)/(1 - v^2/C_0^2)^{1/2}$.

In terms of this variable, Eq. (3.5) is written

$$-\phi_{XX} - \frac{\epsilon k}{C_0^2(1 - v^2/C_0^2)^{3/2}}\phi_X\phi_{XX} + \frac{1}{d^2}(|\phi|-1)\mathrm{sgn}(\phi) = 0 \quad (3.6)$$

($d^2 = C_0^2/\omega_0^2$.) The perturbation term in Eq. (3.6) is proportional to $h = k/C_0^2(1 - v^2/C_0^2)^{3/2}$. Due to the expression of h the first-order perturbation calculation that we use to solve this equation is not appropriate for kinks moving with high velocities since the magnitude of the perturbation term is no longer weak when v approaches C_0. This is easily understood from physical arguments since high velocity kinks are also narrow kinks. Thus the relative displacement of two adjacent particles situated near the kink center is very important. In this limit the cubic terms in the coupling energy bring an important contribution to the strain energy even if $\epsilon \ll 1$. Moreover, in the limit of high velocity kinks ($v \to C_0$ and $d \to l$), even the continuum approximation is no longer valid.

Since we impose the limiting conditions $\phi(X = -\infty) = -1$, $\phi(X = 0) = 0$, and $\phi(X = +\infty) = +1$, Eq. (3.6) is solved by separate studies of the cases $X > 0 (\phi > 0)$ and $X < 0 (\phi < 0)$. In the first case we define the new variable $\Phi(X) = \phi(X) - 1$. Equation (3.6) gives

$$-\Phi_{XX} - \epsilon h\Phi_X\Phi_{XX} + \frac{1}{d^2}\Phi = 0.$$

Multiplying by Φ_X and integrating over X yields

$$-\tfrac{1}{2}\Phi_X^2 - \frac{\epsilon h}{3}\Phi_X^3 + \frac{1}{2d^2}\Phi^2 = C, \quad (3.7)$$

where C is an integration constant. In the limit $X \to +\infty$ we have $\Phi \to 0$ and $\Phi_X \to 0$ so that we obtain $C = 0$. We look for a solution of Eq. (3.7) of the form

$$\Phi = \Phi^0 + \Delta\Phi, \quad (3.8)$$

where $\Phi^0 = -e^{-X/d}$ is solution of the D-Q, M-Q model with harmonic coupling and $\Delta\Phi$ is the kink waveform modification induced by the nonlinear term in the strain energy. We assume that $\Delta\Phi \ll \Phi^0$ ($\Delta\Phi$ is of the order of magnitude of ϵ).

Substitution of Eq. (3.8) into Eq. (3.7) and linearization in $\Delta\Phi$ (or ϵ) gives

$$\frac{\epsilon h}{3}(\Phi_X^0)^3 - \frac{1}{d^2}\Phi^0\Delta\Phi + \Phi_X^0\Delta\Phi_X = 0.$$

Recalling the expression for Φ^0, one obtains the following equation for the deviation of the kink waveform induced by the nonlinear coupling:

$$\Delta\Phi_X + \frac{1}{d}\Delta\Phi = -\tfrac{1}{3}\frac{\epsilon h}{d^2}e^{-2X/d}. \quad (3.9)$$

Equation (3.9) is solved with the limiting conditions $\Delta\Phi(X = 0) = 0$ and $\Delta\Phi(X \to +\infty) = 0$ arising from the general conditions that we impose on the kink solution. The kink waveform is found to be

$$\Phi(X > 0) = -\exp(-X/d) - \frac{\epsilon h}{3d}[\exp(-X/d) - \exp(-2X/d)].$$

[The same method is used to determine Φ in the case $X < 0$.] The modified kink or antikink solution of Eq. (3.6) is finally obtained in the form

$$\phi_s'^{(v)}(X) = \mathrm{sgn}(X)\{\pm[1 - \exp(-|X|/d)] - \frac{\epsilon k}{3dC_0^2(1 - v^2/C_0^2)^{3/2}} \times [\exp(-|X|/d) - \exp(-2|X|/d)]\} \quad (3.10)$$

(in the following we denote by a prime all functions which are relative to the nonlinear coupling case). The sign + refers to the kink while the sign − refers to the antikink. In Fig. 2 we compare the waveform of the modified kink or antikink in the rest frame to the waveform of the kink or antikink with harmonic coupling. It is interesting to notice that the kink and antikink are no longer symmetrical in the presence of the nonlinear coupling term. This result arises from the cubic form of this term, which breaks the symmetry with respect to the change of x into $-x$. Since we solved Eq. (3.6) in a first order approximation, the expression (3.10) is valid only when the modification induced by the nonlinear coupling term is weak. As one would expect from physical arguments, this modification is localized around the center of the kink, where distances between adjacent particles are very different from equilibrium distances so that the contribution of the nonlinear coupling term is maximum. Recalling the value of $X = (x - vt)/(1 - v^2/C_0^2)^{1/2}$ in Eq. (3.10) we note that the kink waveform is not Lorentz covariant. This is related to the noncovariant form of Eq. (3.6). Nevertheless one could obtain the waveform of a modified kink or antikink from the static solution

$$\phi_s'^0(x) = \mathrm{sgn}(x)\{\pm[1 - \exp(-|x|/d)] - \epsilon k/3dC_0^2[\exp(-|x|/d) - \exp(-2|x|/d)]\} \quad (3.11)$$

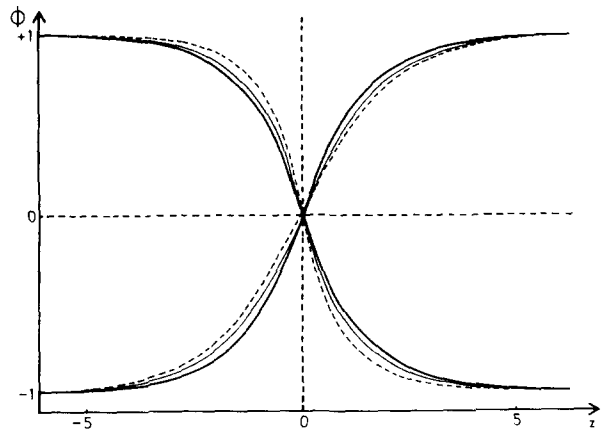

FIG. 2. Comparison between the static kink (antikink) waveform in the harmonically coupled system (heavy line) and the modified kink (antikink) waveforms for two example values of the nonlinear coupling term: $\epsilon k/3d = 0.2$ (thin line) and $\epsilon k/3d = 0.5$ (dotted line).

by first performing a Lorentz transformation upon the coordinates and then changing k into $k/(1-v^2/C_0^2)^{3/2}$. This last transformation is associated with the narrowing of the moving kink which increases the contribution of the nonlinear coupling terms.

IV. GENERALIZED SUSCEPTIBILITY OF THE D-Q AND M-Q CHAINS WITH NONLINEAR COUPLING

In this section we use an extended form of the general formalism,[14,15] reviewed in Sec. II in the case of harmonic coupling, to compute the dynamic polarizability of the D-Q and M-Q kinks in the presence of nonlinear coupling. First we give the equation which governs the linear response of the modified kink described in Sec. III to an external applied field. Before solving this equation we define a new set of functions $\{f'_m\}$ derived from the orthonormal set $\{f_m\}$ introduced in Sec. II, which has been modified to account for the new kink waveform in the presence of nonlinear coupling. Then we obtain a general expression of the response function of the kink in terms of the basis $\{f'_m\}$. The last step is the analytical evaluation of this expression to obtain an explicit form of the response function which is finally Fourier transformed to derive the generalized susceptibility of the chain in the presence of nonlinear coupling.

We consider the effect of an external field $\mathscr{E}(x,t)$ applied to the chain with nonlinear coupling described by Eq. (3.4). We also assume a linear damping $\gamma\partial\phi/\partial t$ as in Sec. II. Thus the displacement field equation of motion is

$$\ddot{\phi} - C_0^2\phi_{xx} - \epsilon k\phi_x\phi_{xx} + \omega_0^2\frac{\partial}{\partial\phi}[V(\phi)] + \gamma\dot{\phi} = \mathscr{E}(x,t) \tag{4.1}$$

and we turn our attention to the study of the response $\Delta\phi'(x,t)$ to the disturbance $\mathscr{E}(x,t)$, superimposed on a static solitary wave $\phi'^0_S(x)$ whose expression is given by Eq. (3.11). Consequently we seek a solution of the form

$$\phi'(x,t) = \phi'^0_S(x) + \Delta\phi'(x,t). \tag{4.2}$$

As in Sec. II we assume that $\Delta\phi'$ is small if $\mathscr{E}(x,t)$ is small in magnitude. Substitution of Eq. (4.2) into Eq. (4.1) gives

$$\begin{aligned}\frac{\partial^2\Delta\phi'}{\partial t^2} &- \frac{d^2\phi'^0_S}{dx^2} - \frac{\partial^2\Delta\phi'}{\partial x^2} \\ &- \epsilon k\left(\frac{d\phi'^0_S}{dx} + \frac{\partial\Delta\phi'}{\partial x}\right)\left(\frac{d^2\phi'^0_S}{dx^2} + \frac{\partial^2\Delta\phi'}{\partial x^2}\right) \\ &+ \gamma\frac{\partial\Delta\phi'}{\partial t} + \frac{\partial}{\partial\phi}[V(\phi'^0_S)] \\ &+ \mathscr{V}(x,t) = \mathscr{E}(x,t),\end{aligned} \tag{4.3}$$

where

$$\mathscr{V}(x,t) = \frac{\partial}{\partial\phi}[V(\phi'^0_S + \Delta\phi')] - \frac{\partial}{\partial\phi}[V(\phi'^0_S)]. \tag{4.4}$$

The determination of $\mathscr{V}(x,t)$ is similar to the corresponding determination which is necessary to compute the small oscillations in the presence of a static kink with harmonic coupling and we find

$$\mathscr{V}(x,t) = [1 - 2d'\delta(x)]\Delta\phi'(x,t), \tag{4.5}$$

where $\delta(x)$ is the Dirac delta function and d' is given by

$$1/d' = 1/d - \epsilon k/3C_2^0 d^2. \tag{4.6}$$

(Note that $1/d'$ is the slope of the modified kink waveform at the point $x=0$ instead of $1/d$ for ordinary kinks.)

As a preliminary step in solving Eq. (4.3) we define a complete set of functions $\{f'_m\}$ which are solutions of

$$\begin{aligned}-C_0^2 f'_{m_{xx}}(x) &- 2d'\omega_0^2\delta(x)f'_m(x) \\ &= (\omega_m^2 - \omega_0^2)f'_m(x).\end{aligned} \tag{4.7}$$

Equation (4.7) is formally identical to the equation governing the small free oscillations in the presence of a kink in Sec. II and its solutions can be expressed by Eq. (2.10) in terms of the new dimensionless variable $z' = x/d'$ accounting for the change of d into d' in the equation. Since it is convenient to go on using the dimensionless variable $z = x/d$ to solve Eq. (4.3), the orthonormal set $\{f'_m\}$ is written in terms of the dimensionless variables introduced in Sec. II.

$$f'_b(z) = \frac{1}{\alpha}\exp(-\alpha|z|), \tag{4.8a}$$

$$f'_{K_-}(z) = \frac{1}{\alpha(\pi)^{1/2}}\sin K_-\alpha z \quad (K_- < 0), \tag{4.8b}$$

$$\begin{aligned}f'_{K_+}(z) = &\frac{1}{\alpha(\pi)^{1/2}(1+K_+^2)^{1/2}} \\ &\times(K_+\cos K_+\alpha z - \sin K_+\alpha|z|) \\ &(K_+ > 0),\end{aligned} \tag{4.8c}$$

where $\alpha = d'/d$ and the coefficient $1/\alpha$ is introduced to normalize the functions f'_m with respect to variable z. Remembering that ϕ'^0_S is a solution of the unperturbed equation of motion, the dimensionless form of Eq. (4.3) is

$$\begin{aligned}\frac{\partial^2\Delta\phi'}{\partial\tau^2} &- \frac{\partial^2\Delta\phi'}{\partial z^2} - \epsilon g\frac{d\phi'^0_S}{dz}\frac{\partial^2\Delta\phi'}{\partial z^2} \\ &- \epsilon g\frac{d^2\phi'^0_S}{dz^2}\frac{\partial\Delta\phi'}{\partial z} + \Gamma\frac{\partial\Delta\phi'}{\partial z} \\ &+ [1 - 2\alpha\delta(z)]\Delta\phi' = E(z,\tau),\end{aligned} \tag{4.9}$$

where $g = k/\omega_0^2 d^3$ and Γ, $E(z,\tau)$ are the dimensionless forms of $\gamma, \mathscr{E}(x,t)$ introduced in Sec. II. In the linearization process used to deduce Eq. (4.9) from Eq. (4.3) the term $\epsilon g(\partial\Delta\phi'/\partial z)(\partial^2\Delta\phi'/\partial z^2)$ has been neglected.

Then Eq. (4.9) is time Fourier transformed to give

$$\begin{aligned}-\Omega^2\Delta\hat{\phi}'(z,\Omega) &- \frac{\partial^2}{\partial z^2}[\Delta\hat{\phi}'(z,\Omega)] \\ &- \epsilon g\frac{d\phi'^0_S(z)}{dz}\frac{\partial^2}{\partial z^2}[\Delta\hat{\phi}'(z,\Omega)] \\ &- \epsilon g\frac{d^2\phi'^0_S(z)}{dz^2}\frac{\partial}{\partial z}[\Delta\hat{\phi}'(z,\Omega)] \\ &+ i\Gamma\Omega\Delta\hat{\phi}'(z,\Omega) + [1 - 2\alpha\delta(z)]\Delta\hat{\phi}'(z,\Omega) \\ &= \hat{E}(z,\Omega).\end{aligned} \tag{4.10}$$

In this equation we replace $\Delta\hat{\phi}'(z,\Omega)$ by its expansion in terms of the orthonormal set $\{f'_m(z)\}$

$$\begin{aligned}\Delta\hat{\phi}'(z,\Omega) &= \int_m \Delta\hat{\phi}'_m(\Omega)f'_m(z) \\ &= \Delta\hat{\phi}'_b + \int_{K_\pm}\Delta\hat{\phi}_{K_\pm}(\Omega)f'_{K_\pm}(z).\end{aligned} \tag{4.11}$$

Making use of the dimensionless form of Eq. (4.7) which is satisfied by the functions f'_m, substitution of Eq. (4.11) into Eq. (4.10) gives the following result:

$$\int_m (\bar{\omega}_m^2 - \Omega^2 + i\Gamma\Omega)\Delta\hat{\phi}'_m f'_m(z) - \epsilon g \int_m \Delta\hat{\phi}'_m \left(\frac{d\phi'^0_S}{dz} \frac{d^2 f'_m}{dz^2} + \frac{d^2\phi'^0_S}{dz^2} \frac{df'_m}{dz} \right) = \int_m \hat{E}_m(\Omega) f'_m(z). \tag{4.12}$$

Equation (4.12) determines the coefficients $\Delta\phi'_m(\Omega)$ in the serie expansion of the response $\Delta\phi'(z,\Omega)$. Since the set $\{f'_m\}$ is an orthonormal basis, multiplying by $f'_n(z)$ and integrating over z gives

$$\Delta\hat{\phi}'_n(\Omega)(\bar{\omega}_n^2 - \Omega^2 + i\Gamma\Omega) - \epsilon g \int_m A(m,n)\Delta\hat{\phi}'_m(\Omega) = \hat{E}_n(\Omega) \tag{4.13}$$

if we define $A(m,n)$ by

$$A(m,n) = \int dz \left(\frac{d\phi'^0_S}{dz} \frac{d^2 f'_m}{dz^2} + \frac{d^2\phi'^0_S}{dz^2} \frac{df'_m}{dz} \right) f'_n(z). \tag{4.14}$$

We now derive a general expression of the response function in the presence of the static kink ϕ'^0_S in terms of these coefficients $A(m,n)$ which will be evaluated later. The major change with respect to the case of harmonic coupling reviewed in Sec. II is that Eq. (4.13) define in fact an infinite system of coupled equations which must be solved to deduce the coefficients $\Delta\hat{\phi}'_n(\Omega)$. Fortunately the term which couples the equations for different values of the index n is a small corrective term (note the factor ϵ) and we can, in a first approach, determine the coefficients $\Delta\hat{\phi}'_n(\Omega)$ by substituting, in the small corrective term, $\Delta\hat{\phi}'_m(\Omega)$ by their value computed with $\epsilon = 0$. It then follows from Eq. (4.13) that

$$\Delta\hat{\phi}'_n(\Omega) = \frac{\hat{E}_n(\Omega)}{\bar{\omega}_n^2 - \Omega^2 + i\Gamma\Omega} + \epsilon g \int_m \frac{A(m,n)\hat{E}_m(\Omega)}{(\bar{\omega}_m^2 - \Omega^2 + i\Gamma\Omega)(\bar{\omega}_n^2 - \Omega^2 + i\Gamma\Omega)}. \tag{4.15}$$

The first term in Eq. (4.15) arises from the harmonic contribution to the coupling between adjacent particles, while the second one arises from the nonlinear coupling term. Substitution of Eq. (4.15) into Eq. (4.11) gives the response $\Delta\hat{\phi}'(z,\Omega)$

$$\Delta\hat{\phi}'(z,\Omega) = \int_n \frac{\hat{E}_n(\Omega)}{\bar{\omega}_n^2 - \Omega^2 + i\Gamma\Omega} f'_n(z) + \epsilon g \int_n f'_n(z) \int_m \frac{A(m,n)\hat{E}_m(\Omega)}{(\bar{\omega}_m^2 - \Omega^2 + i\Gamma\Omega)(\bar{\omega}_n^2 - \Omega^2 + i\Gamma\Omega)}. \tag{4.16}$$

Since the coefficients $\hat{E}_m(\Omega)$ are defined by

$$\hat{E}_m(\Omega) = \int dz' \, \hat{E}(z',\Omega) f'_m(z'),$$

we obtain

$$\Delta\hat{\phi}'(z,\Omega) = \int dz' \, \hat{E}(z',\Omega) \int_n \frac{f'_n(z) f'_n(z')}{(\bar{\omega}_n^2 - \Omega^2 + i\Gamma\Omega)} + \epsilon g \int dz' \, \hat{E}(z',\Omega) \int_n f'_n(z) \times \int_m \frac{A(m,n) f'_m(z')}{(\bar{\omega}_m^2 - \Omega^2 + i\Gamma\Omega)(\bar{\omega}_n^2 - \Omega^2 + i\Gamma\Omega)}. \tag{4.17}$$

A comparison between Eq. (4.17) and Eq. (2.15) which defines the response function of the system gives the following expression for the response function $\alpha'(z,z';\Omega)$ in the presence of nonlinear coupling

$$\alpha'(z,z';\Omega) = \int_n \frac{f'_n(z) f'_n(z')}{\bar{\omega}_n^2 - \Omega^2 + i\Gamma\Omega} + \epsilon g \int_n f'_n(z) \int_m \frac{A(m,n) f'_m(z')}{(\bar{\omega}_m^2 - \Omega^2 + i\Gamma\Omega)(\bar{\omega}_n^2 - \Omega^2 + i\Gamma\Omega)}. \tag{4.18}$$

As we consider only that part of the response corresponding to the deformation of the kink waveform (i.e., we do not study the central peak), we drop the term $n = b$ from the n sum in Eq. (4.17). The generalized summation in which the term $n = b$ is excluded is denoted by $\int'_n$. The first term in Eq. (4.18) which is formally identical to the response function obtained in Sec. II is the contribution to the response function arising from the harmonic-coupling term in the strain energy. Its value is given by Eq. (2.17) and we now concentrate on the second term in Eq. (4.17), henceforth denoted by $\Delta\alpha(z,z';\Omega)$, which describes the modification of the response function induced by the nonlinear coupling.

The calculation of the explicit form of $\Delta\alpha(z,z';\Omega)$ from Eq. (4.18) is performed in two steps. The first step is the calculation of coefficients $A(m,n)$ and the second one consists in the integrations over m and n. We now examine successively these two steps.

The coefficients $A(m,n)$ are defined by Eq. (4.14) and, since we have dropped $n = b$ from the n sum in Eq. (4.18) we have only to calculate $A(m,n)$ with $n \neq b$. Recalling the expression of ϕ'^0_S given by the dimensionless form of Eq. (3.11) we have

$$\frac{d\phi'^0_S}{dz} = \exp(-|z|) + \epsilon k/3d \, [\exp(-|z|) - 2\exp(-2|z|)] \tag{4.19a}$$

and

$$\frac{d^2\phi'^0_S}{dz^2} = -\operatorname{sgn}(z)\{\exp(-|z|) + \epsilon k/3d \times [\exp(-|z|) - 4\exp(-2|z|)]\}. \tag{4.19b}$$

Note that $d\phi'^0_S/dz$ is an even function of z while $d^2\phi'^0_S/dz^2$ is an odd function of z. Thus to compute $A(m,n)$ from Eq. (4.14) we have to calculate integrals of the form

$$I_1 = \int_{-\infty}^{+\infty} dz \exp(-a|z|) \frac{d^2 f'_m(z)}{dz^2} f'_n(z)$$

and

$$I_2 = \int_{-\infty}^{+\infty} dz \operatorname{sgn}(z) \exp(-b|z|) \frac{df'_m(z)}{dz} f'_n(z),$$

where a and b are constants ($a,b = 1$ or 2), for the different cases $m = b, K_-, K_+$. From simple considerations about the parity of the functions f'_m and of their derivatives it is easy to show that some integrals of the I_1 or I_2 type vanish so that we deduce

$$A(b,n) = 0 \text{ for all values of } n\ (n \neq b), \tag{4.20a}$$

$$A(K_-,K'_+) = A(K_+,K'_-) = 0 \text{ for all } K_- < 0 \text{ and } K_+ > 0. \tag{4.20b}$$

Consequently the only nonvanishing $A(m,n)$ terms are of the form $A(K_-,K'_-)$ $(K_-,K'_- < 0)$ or $A(K_+,K'_+)$ $(K_+,K'_+ > 0)$. Upon making use of Eqs. (4.14), (4.19), and (4.8) and performing the z integrations we obtain

$$A(K_-,K'_-) = -\frac{K_-K'_-}{\pi}\left\{\frac{1}{1+(K_-+K'_-)^2\alpha^2} + \frac{1}{1+(K_--K'_-)^2\alpha^2}\right\} \tag{4.21a}$$

and

$$A(K_+,K'_+) = \frac{1}{\alpha\pi\sqrt{1+K_+^2}\sqrt{1+K_+'^2}} \times\left\{\frac{\alpha^2K_+^2(K_++K'_+)^2+\alpha K_+^2K_+'^2-\alpha K_+K'_++K_+(K_++K'_+)}{1+(K_++K'_+)^2\alpha^2} - \frac{\alpha^2K_+^2(K_+-K'_+)^2+\alpha K_+^2K_+'^2+\alpha K_+K'_++K_+(K_+-K'_+)}{1+(K_+-K'_+)^2\alpha^2}\right\}. \tag{4.21b}$$

Once all the coefficients $A(m,n)$ $(n \neq b)$ are evaluated the next step is to perform the generalized summations $\int'_n$ and $\int'_m$ in Eq. (4.18). This calculation is still separated into two steps. We first compute

$$F_n(z') = \int'_m \frac{A(m,n)f'_m(z')}{\bar{\omega}_m^2 - \Omega^2 + i\Gamma\Omega} \tag{4.22}$$

and then integrate over n

$$\Delta\alpha(z,z';\Omega) = \epsilon g\int'_n \frac{F_n(z')f'_n(z)}{\bar{\omega}_n^2 - \Omega^2 + i\Gamma\Omega}. \tag{4.23}$$

Consider first the calculation of $F_{K'_+}(z')$ $(n = K'_+ > 0)$. According to Eq. (4.20), only the terms with $m = K_+ (K_+ > 0)$ contribute so that we obtain

$$F_{K'_+}(z') = \int_0^{+\infty} dK_+ \frac{A(K_+,K'_+)}{\alpha^2K_+^2 - Q^2} f'_{K_+}(z'), \tag{4.24}$$

where we have used the dispersion relation $\bar{\omega}_K^2 = 1 + \alpha^2K^2$ and we have defined $Q^2 = \Omega^2 - 1 - i\Gamma\Omega$. After substitution of Eq. (4.21b) into Eq. (4.24) and after some simplifications arising from parity considerations $F_{K'_+}(z')$ may be written

$$F_{K'_+}(z') = \frac{(1-\alpha)K'_+}{\alpha^2\pi^{3/2}\sqrt{1+K'^2_+}} \int_{-\infty}^{+\infty} dK_+ \frac{K_+f_{K_+}(z')}{(\alpha^2K_+^2 - Q^2)[1+(K_+-K'_+)^2\alpha^2](1+K_+^2)}. \tag{4.25}$$

The product $K_+f_{K_+}(z)$ is an even function of K_+ so that the integral over K_+ does not vanish. However, remembering that $\alpha = d'/d$ with $1/d' = 1/d - \epsilon k/3d^2$, this indicates that $\alpha - 1$ is of the order of magnitude of $\epsilon k/3d$. Thus $F_{K'_+}(z)$ is of the order of magnitude of ϵ and due to the factor ϵg in Eq. (4.23) the corresponding contribution to $\Delta\alpha(z,z';\Omega)$ is of the order of magnitude of ϵ^2. Since we perform all our calculations up to the first order in ϵ we must drop this contribution from $\Delta\alpha$. Thus the only contribution to $\Delta\alpha$ which is first order in ϵ arises from the case $n = K_-(K_- < 0)$, and from Eqs. (4.20b), (4.22), and (4.23) we obtain

$$\Delta\alpha(z,z';\Omega) = \epsilon g\int_{-\infty}^{0} dK_-\int_{-\infty}^{0} dK'_- \times \frac{A(K_-,K'_-)f'_{K_-}(z')f'_{K'_-}(z)}{(\alpha^2K_-^2 - Q^2)(\alpha^2K'^2_- - Q^2)}. \tag{4.26}$$

To perform the integrations over K_- and K'_- by means of the residue theorem it is convenient to obtain a more symmetric form of $\Delta\alpha$ in which K_- and K'_- vary between $-\infty$ and $+\infty$. This is achieved by parity considerations and after substitution of Eq. (4.21a) into Eq. (4.26), $\Delta\alpha(z,z';\Omega)$ may be written

$$\Delta\alpha(z,z';\Omega) = -\frac{\epsilon g}{4\pi^2\alpha^2}\int_{-\infty}^{+\infty} dK_-\int_{-\infty}^{+\infty} dK'_- \times \frac{K_-K'_-\sin K'_-\alpha z\sin K_-\alpha z'}{(K_-^2\alpha^2 - Q^2)(K'^2_-\alpha^2 - Q^2)} \times\left\{\frac{1}{1+(K_-+K'_-)^2\alpha^2} + \frac{1}{1+(K'_--K_-)^2\alpha^2}\right\}. \tag{4.27}$$

Thus we have derived an expression of $\Delta\alpha(z,z';\Omega)$ which is more explicit than the general expression (4.18). The last step in the computation of the response function is to perform the integrations over K_- and K'_- in Eq. (4.27). After a tedious calculation we obtain

$$\Delta\alpha(z,z';\Omega) = \mathrm{sgn}(z)\mathrm{sgn}(z')\frac{\epsilon g}{4\alpha^6} \times\left\{\frac{Q+i}{2Q+i}\left[(e^{-|z|}+e^{-|z'|})\times e^{iQ(|z|+|z'|)} - e^{-1/2(|z-z'|+|z+z'|)}e^{iQ||z|-|z'||}\right] + \frac{Q-i}{2Q-i}e^{-1/2||z+z'|-|z-z'||}e^{iQ||z|-|z'||} - \left(1+\frac{1}{1+4Q^2}\right)e^{iQ(|z|+|z'|)}\right\}, \tag{4.28}$$

where Q has the same meaning as in Eq. (2.17). (Q denotes the branch of $(\Omega^2 - 1 - i\Gamma\Omega)^{-1/2}$ having a positive imaginary part.) It is important to notice that setting $z' = z$ and letting

$|z|$ tend to infinity in Eq. (4.28) yields the result

$$\lim_{|z|\to\infty} \Delta\alpha(z,z;\Omega) = 0. \tag{4.29}$$

Equation (4.29) means that the variation of the response induced by the nonlinear coupling term is *localized around the center* ($z = 0$) *of the kink*. Thus the introduction of the nonlinear coupling term only modifies the intrinsic response of the kink and not that part of the total response which is the response of the system in the absence of a kink. In other words, in the absence of a kink the nonlinear coupling term does not modify the response of the system (at least in the framework of the linear response theory, i.e., if we limit the calculations to the first order in ϵ.) This last result can be derived directly from the general equation of motion (4.1). If we look for the response of the system in the absence of a kink we assume a solution of the form

$$\phi''(x,t) = \phi_0'' + \Delta\phi''(x,t) \tag{4.30}$$

instead of (4.2), where $\phi_0'' = \pm 1$ represents the equilibrium positions of the particles in the absence of a kink. If we substitute Eq. (4.30) into (4.1), after linearization in $\Delta\phi''$ the term in ϵk arising from the nonlinear coupling vanishes since $d\phi_0''/dx = 0$, $d^2\phi_0''/dx^2 = 0$ and we neglect $(\partial\Delta\phi''/\partial x)(\partial^2\Delta\phi''/\partial x^2)$ in the linearization process.

Consequently Eq. (4.28) shows that *the presence of a kink enhances the effects of the nonlinear coupling term*; the change in the response function is one order of magnitude higher (with respect to the magnitude ϵ of the perturbation) in the presence of kinks. This is easily understood physically since the presence of kinks induces large displacements from equilibrium positions. This was the reason why it seemed to us particularly interesting to introduce nonlinear coupling in a system bearing kinks due to the existence of a nonlinear substrate potential.

The generalized susceptibility of the system (Eq. 2.18) is the Fourier transform of the response function. Since we have obtained

$$\alpha'(z,z';\Omega) = \alpha(z,z';\Omega) + \Delta\alpha(z,z';\Omega),$$

where α is the response function in the case of harmonic coupling, the generalized susceptibility with nonlinear coupling in the presence of a static kink is

$$\chi'^{(0)}(p,q;\Omega) = \chi^{(0)}(p,q;\Omega) + \Delta\chi^{(0)}(p,q;\Omega). \tag{4.31}$$

The generalized susceptibility of the harmonically coupled system, $\chi^{(0)}(p,q;\Omega)$ is given by Eq. (2.19) and $\Delta\chi^{(0)}(p,q;\Omega)$, which is the Fourier transform of $\Delta\alpha(z,z';\Omega)$, represents the nonlinear coupling contribution to the susceptibility. Since $\Delta\alpha(z,z';\Omega)$ is symmetrical with respect to the permutation of z and z' the Fourier transform is also symmetrical in p and q. Moreover, since $\Delta\alpha$ is an odd function of z and z', $\Delta\chi^{(0)}(p,q;\Omega)$ vanishes for $p = 0$ or $q = 0$. Performing the Fourier transform we obtain

$$\begin{aligned}\Delta\chi^{(0)}(p,q;\Omega) = \epsilon kpq \Bigg\{ & -\frac{Q+i}{2Q+i}\left[\frac{1}{(q^2-Q^2)[(1-iQ)^2+p^2]} + \frac{1}{(p^2-Q^2)[(1-iQ^2)+q^2]}\right] \\ & + \frac{Q+i}{2Q+i}\times\frac{1}{(1+p^2+q^2)^2-4p^2q^2} \\ & \times\left[\frac{3+p^2-q^2-2iQ}{(1-iQ)^2+q^2} + \frac{3+q^2-p^2-2iQ}{(1-iQ)^2+p^2}\right] \\ & - \frac{Q-i}{2Q-i}\times\frac{1}{(1+p^2+q^2)^2-4p^2q^2} \\ & \times\left[\frac{1+p^2-q^2-2iQ}{q^2-Q^2} + \frac{1+q^2-p^2-2iQ}{p^2-Q^2}\right] \\ & + \left(1+\frac{1}{1+4Q^2}\right)\times\frac{1}{(p^2-Q^2)(q^2-Q^2)}\Bigg\}. \end{aligned} \tag{4.32}$$

In Fig. 3 we have plotted the real and imaginary parts of $\Delta\chi^{(0)}(p,p;\Omega)$ for $p = 0.4$ and for a magnitude of the nonlinear term given by $\epsilon k = 0.05$. The magnitude of $\Delta\chi$ increases as p or q increases but it must be remembered that the continuum approximation requires the small wavevectors limit.

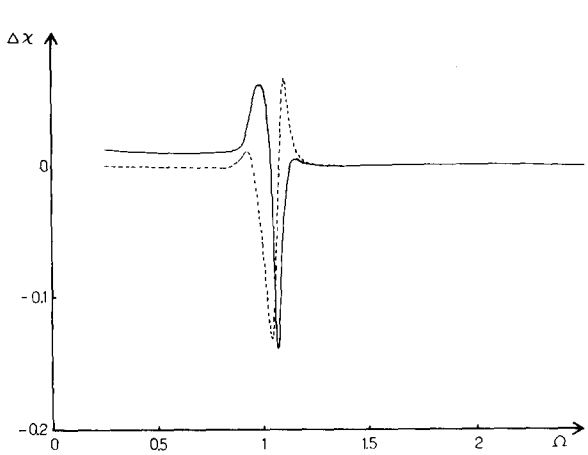

FIG. 3. Nonlinear coupling contribution to the susceptibility $\Delta\chi^{(0)}(p,p;\Omega)$ in the presence of a static kink. The real and imaginary part of $\Delta\chi$ are plotted as solid and dashed curves, respectively.

V. SUMMARY

The main purpose of this paper was to show that it is interesting to introduce coupling nonlinearities in systems bearing kinks. We have shown that, for the D-Q or M-Q models, they can be treated analytically at least in the framework of a first order perturbation theory. We have calculated the modified kink waveform in the presence of cubic nonlinear coupling terms in the Hamiltonian and the contribution to the response function and susceptibility of these nonlinear terms has been determined. The outstanding result is that the existence of a nonlinear substrate potential enhances the effects of coupling nonlinearities; in the presence of kinks nonlinear coupling terms contribute to the first-order term in the perturbation expansion of the susceptibility instead of the second-order one. However, since calculations were performed in the continuum limit, large relative displacements of adjacent particles are excluded and this prevents the coupling nonlinearities from playing the major role that they are expected to play in real systems bearing kinks. Nevertheless our results suggest that it would be very interesting to apply the same calculations to a discrete model bearing narrow kinks.

ACKNOWLEDGMENTS

The author would like to thank Professor M. Remoissenet for many helpful discussions and a critical reading of the manuscript.

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Electrostatic structural transitions in a Gaussian Wigner solid

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(Received 22 June 1981; accepted for publication 11 August 1981)

A derivation is supplied for a functional relation between the Fuchs energy ϵ and the Madelung energy S for a Gaussian Wigner solid (GWS) in which the usual uniform background of a Wigner solid (WS) is replaced by a periodic array of Gaussians with variable "ripple" parameter p allowing the WS and the empty lattice in the limits of small p and large p, respectively. It is the zeros of $\Delta\epsilon$, and not of ΔS, that are relevant for structural transitions between two lattices. Much can be determined about the transitions with minimal computations by utilizing a modest amount of information about order relations on certain theta functions. With increasing p, the sequence of lowest-energy structures restricted to the cubics is bcc, fcc, and sc. A later report will treat the Yukawa WS (YWS) in which the Gaussians are replaced with Yukawa distributions. The functional relation is again derivable, and it is not given by Medeiros and Mokross's recent assumption that $2\epsilon^{\mathrm{YWS}} = S^{\mathrm{YWS}}$.

PACS numbers: 64.70.Kb, 61.50.Lt, 71.45.Nt, 71.10. + n

I. INTRODUCTION

A Wigner[1] solid (WS) is a model composed of point charges Q (of either sign) on a Bravais lattice with a uniform neutralizing background. This is the first of a two-part report on generalized WS's in which the background is modified with variable "ripple" in the charge. This first paper treats the Gaussian WS (GWS) in which the background is formed by centering about each lattice site the charge distribution $-Q(p/\pi)^{3/2}\exp(-pr^2)$. The second will treat the Yukawa WS (YWS) in which $-Q(\lambda^2/4\pi)r^{-1}\exp(-\lambda r)$ is centered similarly. Both of these possess the WS and the empty lattice as limiting cases. The purpose of these papers is to supply derivations of the Fuchs energy ϵ, the Madelung energy S, and functional relations between these two energies. Recently, I reported[2] the final results for the GWS and the YWS, applied them to the cubic lattices, and pointed out that Medeiros and Mokross[3] have incorrectly assumed that $2\epsilon^{\mathrm{YWS}} = S^{\mathrm{YWS}}$. Quite stringent tests satisfied by the final results add confidence in the validity of the derivations.

The Fuchs energy ϵ, which will be defined in Eq. (26), is the interaction energy of all charge normalized to the volume Ω occupied by each point charge Q, and it is the relevant quantity for determining which of two lattices is preferred energetically. It is generally more difficult to calculate than the Madelung energy S, defined by Eqs. (3) and (10), which is given by $S = K - A$, $A = Q\langle\Phi\rangle$, where $\langle\Phi\rangle$ is the average potential of all charge and K is the energy of interaction between one point charge Q and all other charge. If one momentarily ignores the difference between K and S, and if one recalls results for simple non-Coulombic models like the Lennard–Jones solids, one might expect $2\epsilon = S$ as is the case for the WS. However, doubt would be cast on this expectation by considering the classical Coulomb lattice (CCL) model[4] composed of one lattice of point charges Q and another identical displaced lattice of point charges $-Q$ for which $\epsilon^{\mathrm{CCL}} = S^{\mathrm{CCL}}$. For two lattices with the same Ω it is the zeros of $\Delta\epsilon$, and not of ΔS, as a function of the ripple parameter p (or λ) that determine where transitions occur. As Ref. 2 and Fig. 1 show, the set of zeros of $\Delta\epsilon$ and the set of zeros for ΔS differ even in number in general.

The WS model has been found useful in many theories (solid state, plasma, low temperature, and pulsars) as discussed by several authors.[5–9] Generalizations of the WS that change either the uniform background or the lattice of point charges Q offer a wider range from which to select more realistic models. Reference 3 used the YWS to represent phase transitions in systems formed by polystyrene particles in aqueous suspensions as observed by Williams *et al.*,[10] and

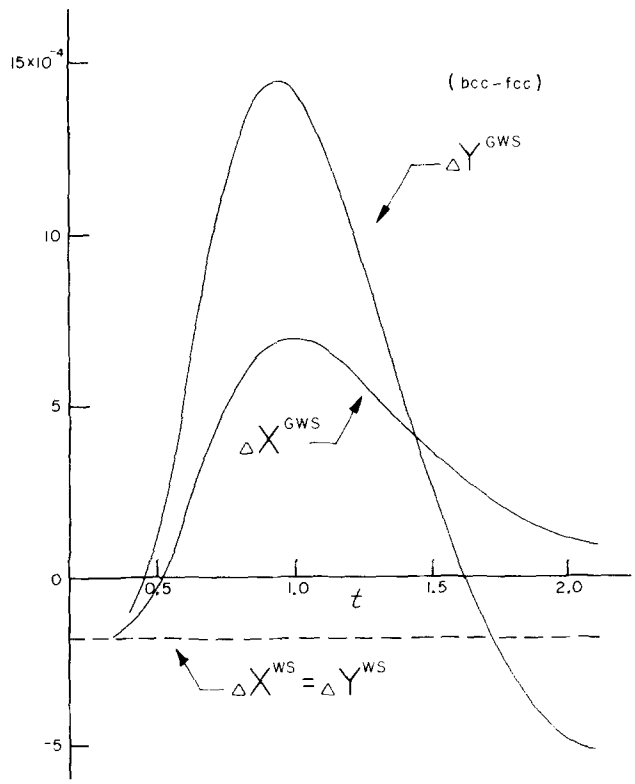

FIG. 1. Comparison of the (bcc-fcc) differences for the Madelung ($S = FX$) and twice the Fuchs ($2\epsilon = FY$) energies reduced by $F = Q^2/\Omega^{1/3}$ as a function of the "ripple" parameter $t = p(\Omega^{2/3}/\pi)$ for the Gaussian (GWS) Wigner solids. Zeros of ΔY^{GWS} locate transitions.

 0022-2488/81/122996-06$01.00

Birman[11] has used Gaussians in various ways to try to improve upon the CCl as a model for ionic crystals. Most generalizations of the WS present considerable complications in the reduction of complicated defining expressions for ϵ to simple forms and in the search for functional relations between ϵ and S. The present derivations for the GWS and those to be presented later for the YWS serve as prototypes, presenting slightly different mathematical difficulties and leading to different functional relations.

To express extra difficulties encountered for the GWS and YWS over those for the WS, consider lattice summations and cellular integrations as "summations." Then for the WS one starts with a defining expression for ϵ^{WS}, part of which involves a sequence of twelve summations, and reduces it to an expression with three summations. For the GWS and YWS I start with defining expressions involving a sequence of eighteen summations and reduce them to a sequence of three summations.

The calculations involve limiting processes which must be performed with consistent account of the arbitrariness of the average potential and with care to avoid errors generated through unjustified interchange of the order of summation and integration in Ewald procedures. My derivations of ϵ^{GWS} and ϵ^{YWS} parallels that for ϵ^{WS} given by Hall and Rice[12] beginning with their Eq. (6). To investigate ϵ one needs to develop expressions for $K(\mathbf{r})$ and $S(\mathbf{r})$ generalized beyond those of Ref. 12 through the more general potential $\Phi(\mathbf{r})$, where $K = K(\mathbf{0})$ and $S = S(\mathbf{0})$. These can be defined without recourse to Ewald techniques, namely by

$$\Phi(\mathbf{r}) = \langle \Phi \rangle + S(\mathbf{r})/Q + Q/r, \tag{1}$$

$$K(\mathbf{r}) = S(\mathbf{r}) + A, \quad A = Q\langle \Phi \rangle, \tag{2}$$

$$S = \lim_{r\to 0} S(\mathbf{r}) = \lim_{r\to 0} Q[\Phi(\mathbf{r}) - \langle \Phi \rangle - Q/r]. \tag{3}$$

Once the $\Phi(\mathbf{r})$ is defined for a model, the $K(\mathbf{r})$ and $S(\mathbf{r})$ are defined. The $\Phi(\mathbf{r})$, $K(\mathbf{r})$, K, and A are multivalued, but $S(\mathbf{r})$, S and ϵ are unique. Until recently errors were made in applications of Ewald techniques which were equivalent to incorrectly equating K and S in the theory of S and equating $K(\mathbf{r})$ and $S(\mathbf{r})$ in the theory of ϵ; Hall[13] uncovered the first error and Ihm and Cohen[14] uncovered the second for the WS case. The canceling effect of these two errors for the WS has been discussed.[12,14] The related matter of why Evjen[15] encountered "Evjen oscillations" in his use of direct summation methods for the CCL model of CsCl but not for NaCl has also been discussed briefly in Ref. 12.

I shall develop in Sec. II various ways of expressing $K(\mathbf{r})$ and $S(\mathbf{r})$, needed in Sec. III, and discuss the evaluation of ΔS for a broad class of pairs of lattices. In Sev. III I reduce the defining expression for ϵ to a simple form convenient for evaluation and from which a functional relation between ϵ and S is derivable. Section IV treats the functional relation.

II. EXPRESSION FOR $K(\mathbf{r})$ AND $S(\mathbf{r})$ FOR THE GWS

Denote with $\{\tau\}$ a Bravais lattice with volume Ω per lattice point. Denote with $\{\gamma\}$ its reciprocal lattice normalized by $\exp(i\gamma\cdot\tau) = 1$. The charge distribution for the GWS is then given by

$$\rho(\mathbf{r}) = Q\sum_{\tau}\left\{\delta(\mathbf{r}-\tau) - \left(\frac{p}{\pi}\right)^{3/2}\exp[-p(\mathbf{r}-\tau)^2]\right\} \tag{4}$$

$$= Q\sum_{\gamma}{}'\left[1 - \exp\left(-\frac{\gamma^2}{4p}\right)\right]\exp(i\gamma\cdot\mathbf{r}), \tag{5}$$

which is well defined in the sense of tempered distributions[16] for all $0 \leqslant p < \infty$. As p approaches zero and infinity, the WS model and the empty lattices are secured, respectively.

To secure the potential $\Phi(\mathbf{r})$ one might consider starting with $\nabla^2\Phi(\mathbf{r}) = -4\pi\rho(\mathbf{r})$, using Fourier series, and writing

$$\Phi(\mathbf{r}) = \langle \Phi \rangle + \frac{4\pi Q}{\Omega}\sum_{\gamma}{}'\left[\frac{1-\exp(-\gamma^2/4p)}{\gamma^2}\right]\exp(i\gamma\cdot\mathbf{r}), \tag{6}$$

but this has two shortcomings. First, it gives no indication of how the average potential may be defined in terms of $\rho(\mathbf{r})$ and the sequence of "summation cells" used[12] to define the potential for an infinite array of charge. Second, the sum in Eq. (6) converges conditionally, giving ambiguity other than that contained in $\langle \Phi \rangle$. To avoid these ambiguities, we need to display the limiting process by which $\Phi(\mathbf{r})$ and $K(\mathbf{r})$ are defined, which are arbitrary only via the arbitrariness of the average potential.

It is only necessary that $\langle \Phi \rangle$ be treated equivalently everywhere. For definiteness, choose a summation cell[12] for defining $\Phi(\mathbf{r})$ to be the proximity cell of the τ lattice and imagine a finite array of these cells centered on lattice sites. Let each cell contain the charge that a similar cell contains in the infinite charge array. The charge in each cell will have reflection symmetry (no dipole moment), and a finite array of them will possess a well defined potential if a point charge is taken to contribute a potential going as r^{-1}. The limit of an infinite nested sequence of these finite arrays, defines the total potential $\Phi(\mathbf{r})$ such that $\langle \Phi \rangle$ is given by Eq. (5) of Ref. 12, which we do not need explicitly here. With this limiting processes understood on the τ summation, Eq. (2) gives

$$\frac{K(\mathbf{r})}{Q^2} = \lim_{N\to\infty}\sum_{\tau}^{N}{}'\left\{\frac{1}{|\mathbf{r}-\tau|} - \int_{\tau}\sum_{\tau'}^{\infty}\left(\frac{p}{\pi}\right)^{3/2}\frac{\exp[-p(\mathbf{z}-\tau')^2]}{|\mathbf{z}-\mathbf{r}|}\right\}d^3z - \int_0\sum_{\tau'}^{\infty}\left(\frac{p}{\pi}\right)^{3/2}\frac{\exp[-p(\mathbf{z}-\tau')^2]}{|\mathbf{z}-\mathbf{r}|}d^3z, \tag{7}$$

$$= \lim_{N\to\infty}\sum_{\tau}^{N}{}'\left\{\frac{1}{|\mathbf{r}-\tau|} - \frac{1}{\Omega}\int_{\tau}\sum_{\gamma}^{\infty}\frac{\exp[-(\gamma^2/4p)+i\gamma\cdot\mathbf{z}]}{|\mathbf{z}-\mathbf{r}|}d^3z\right\} - \frac{1}{\Omega}\int_0\sum_{\gamma}^{\infty}\frac{\exp(-\gamma^2/4p)\exp(i\gamma\cdot\mathbf{z})}{|\mathbf{z}-\mathbf{r}|}d^3z, \tag{8}$$

$$= \lim_{N\to\infty}\sum_{\tau}^{N}{}'\int_0^{\infty}\frac{1}{(\pi\nu)^{1/2}}\{\exp[-\nu(\tau-\mathbf{r})^2] - \frac{1}{\Omega}\int_{\tau}\sum_{\gamma}^{\infty}\exp\left[-\left(\frac{\gamma^2}{4p}\right)+i\gamma\cdot\mathbf{z}-(\mathbf{z}-\mathbf{r})^2\nu\right]d^3z\}d\nu$$

$$-\frac{1}{\Omega}\int_0^{\infty}\frac{1}{(\pi\nu)^{1/2}}\int_0\sum_{\gamma}^{\infty}\exp\left[-\left(\frac{\gamma^2}{4p}\right)+i\gamma\cdot\mathbf{z}-(\mathbf{z}-\mathbf{r})^2\nu\right]d^3zd\nu, \tag{9}$$

where the Poisson summation formula (PSF)[17] is used to secure Eq. (8) and the lemma of Eq. (A3) of Ref. 13 is used to get Eq. (9). As analyzed in Ref. 13, passing the τ summation inside the integral in Eq. (9) brings in the average potential such that $K(\mathbf{r}) = S(\mathbf{r}) + A$ and

$$\frac{S(\mathbf{r})}{Q^2} = \int_0^\infty \frac{1}{(\pi\nu)^{1/2}} \left\{ \sum_\tau{}' \exp[-\nu(\tau-\mathbf{r})^2] - \frac{1}{\Omega}\left(\frac{\pi}{\nu}\right)^{3/2} \sum_\gamma \exp\left\{ -\left[\frac{\gamma^2(p+\nu)}{4p\nu} + i\gamma\cdot\mathbf{r} \right] \right\} \right\} d\nu, \tag{10}$$

$$= \int_0^\infty \frac{1}{\sqrt{\pi\nu}} \left\{ \sum_\tau{}' \exp[-\nu(\tau-\mathbf{r})^2] - \left(\frac{p}{p+\nu}\right)^{3/2} \sum_\tau \exp\left[-\left(\frac{p\nu}{p+\nu}\right)(\mathbf{r}-\tau)^2 \right] \right\} d\nu, \tag{11}$$

$$= \int_0^\infty \frac{1}{\sqrt{\pi\nu}} \left(-\exp(-\nu r^2) + \frac{1}{\Omega}\left(\frac{\pi}{\nu}\right)^{3/2} \sum_\gamma \left\{ \exp\left(\frac{-\gamma^2}{4\nu}\right) - \exp\left[-\frac{\gamma^2(p+\nu)}{4p\nu} \right] \right\} \exp(i\gamma\cdot\mathbf{r}) \right) d\nu. \tag{12}$$

This variety of expressions for $S(\mathbf{r})$ is needed for various integrals of $K(\mathbf{r})$ or $S(\mathbf{r})$ and for various limits on $S(\mathbf{r})$ and $S = S(\mathbf{0})$. Through the Eqs. (1)–(3), they also provide a variety of expressions for $\Phi(\mathbf{r})$.

By setting r and p equal to zero in Eqs. (10) and (12) to secure expressions for S^{WS} and then using the integrand of Eq. (10) over the domain $0 < d \leqslant v < \infty$ and the integrand of Eq. (12) over $0 \leqslant v \leqslant d$, one can express S^{WS} as the sum of two rapidly converging sums. This is called the Ewald theta function method (TFM),[18] because both integrands are types of theta functions (TF's). In the sequel TF's will be used in additional ways, mostly utilizing an earlier report[19] of order relations on TF's.

For p smaller than about $3\pi/2\Omega^{2/3}$ it is convenient to write

$$S(\mathbf{r}) = S^{\mathrm{WS}}(\mathbf{r}) - \frac{4\pi Q^2}{\Omega} \int_{1/4p}^\infty \sum_\gamma{}' \exp(-u\gamma^2 + i\gamma\cdot\mathbf{r})\, du \tag{13}$$

$$= S^{\mathrm{WS}}(r) - \frac{4\pi Q^2}{\Omega} \sum_\gamma{}' \frac{\exp[-(\gamma^2/4p) + i\gamma\cdot\mathbf{r}]}{\gamma^2} \tag{14}$$

found from Eq. (12) by properly grouping terms to separate S^{WS} and then setting $v = 1/4u$. These two show clearly that $S(\mathbf{r})$ approaches $S^{\mathrm{WS}}(\mathbf{r})$ as p approaches zero. Another important check on my expressions for $S(\mathbf{r})$ is given by the empty lattice limit of p approaching infinity. From Eq. (11) it is seen that

$$S(\mathbf{r}) \sim -Q^2 \int_0^\infty \frac{1}{(\pi\nu)^{1/2}} \left(\frac{p}{p+\nu}\right)^{3/2} \exp\left[-r^2\left(\frac{p\nu}{p+\nu}\right) \right] d\nu, \tag{15}$$

$$S \sim -Q^2 \int_0^\infty \frac{1}{(\pi\nu)^{1/2}} \left(\frac{p}{p+\nu}\right)^{3/2} d\nu = -2Q^2 \left(\frac{p}{\pi}\right)^{1/2}. \tag{16}$$

This last result checks with what one can calculate directly as the leading contribution to K, hence S, from the interaction between Q and the local background as the local background near a point charge Q "bunches" up to become a point charge $-Q$. Since this leading term is structure independent, it cancels in the difference between the S's for two lattices with the same Ω.

Properties of ΔS for two lattices

In studying $\Delta\epsilon$ for two lattices to see which lattice provides the lower energy structure, it is convenient to express $\Delta\epsilon$ in terms of ΔS; both are expressible in terms of ΔS^{WS} and a function H depending on TF's. A study of the zeros of ΔS and $\Delta\epsilon$ then reduces to a study of H for which a knowledge of order relations[19] on TF's permits one to determine a great deal about H and the zeros without numerical work. Then further details follow from a modest amount of computation. Although the numerical results reported[2] for the bcc-fcc, fcc-sc, and bcc-sc systems might appear to be a bit specialized, they actually provide prototypical results for a broad class of pairs of lattices. From the role of order relations on TF's it can be seen that the results for, say, the fcc-sc system are qualitatively similar to those for the fcc-hcp system; the hcp (hexagonal close packed) is not a Bravais lattice, but all the equations of this paper are easily modified to apply to such lattices. All of this becomes most transparent in terms of reduced energies and unit (volume) lattices.

Define mutually-reciprocal, unit lattices (a,b) by $\tau = \Omega^{1/3}\mathbf{a}, \gamma = 2\pi\mathbf{b}/\Omega^{1/3}$, and $\exp(2\pi i\mathbf{a}\cdot\mathbf{b}) = 1$. When one wants to compare the energies above for two lattices either when the two are reciprocally related (bcc-fcc) or not (fcc-sc or fcc-hcp), the unit lattices reduce the need for notation and permit utilization of any reciprocity.

First consider two competing lattices that are mutually reciprocal and such that the a lattice has a shorter first-neighbor distance than the b. As prototypes, identify the bcc with the a lattice and the fcc with the b. Also define $S = FX$, $F = Q^2/\Omega^{1/3}$, and $\Delta X = X(a) - X(b)$. Then with $r = 0$, Eqs. (13) and (14) give $\Delta X = \Delta X^{\mathrm{WS}} + H(t)$, with $t = p\Omega^{2/3}/\pi$, $H(\infty) = -\Delta X^{\mathrm{WS}}$, and

$$H(t) = \int_{1/t}^\infty \left[\sum_a{}' \exp(-\pi s a^2) - \sum_b{}' \exp(-\pi s b^2) \right] ds \tag{17}$$

$$= \sum_a{}' \frac{\exp(-\pi a^2/t)}{\pi a^2} - \sum_b{}' \frac{\exp(-\pi b^2/t)}{\pi b^2}. \tag{18}$$

The integrand of Eq. (17) is equal to the difference between two TF's, namely, $N_a(s) - N_b(s)$ in the notation of Ref. 19, so it may be expressed as $\Delta N(s)$. Any (a,b) system obeying the order relations reported[19] for the bcc-fcc system will possess an $H(t)$ with the properties I now outline for the bcc-fcc system.

In terms of N the order relations are

$$N_{\mathrm{sc}}(s) > N_{\mathrm{bcc}}(s), N_{\mathrm{fcc}}(s) \quad 0 < s < \infty, \tag{19}$$

$$N_{\mathrm{fcc}}(s) > N_{\mathrm{bcc}}(s) \quad 0 < s < 1, \tag{20}$$

$$N_{\mathrm{bcc}}(s) > N_{\mathrm{fcc}}(s) \quad 1 < s < \infty. \tag{21}$$

The curves of the three cubic N's become asymptotically

equal as s approaches zero or infinity, and $N_{fcc}(1) = N_{bcc}(1)$. Thus $\Delta N(s)$ is negative for $0 < s < 1$ and positive for $1 < s < \infty$. Since the lower limit of integration in Eq. (17) is $1/t$, $H(0) = 0$ and $H(t)$ increases to a maximum at $t = 1$. Beyond $t = 1$ the $H(t)$ decreases but remains positive, because the magnitude of the integral of $\Delta N(s)$ from $0 \leqslant s \leqslant 1$ is less than the integral from $1 \leqslant s \leqslant \infty$, as follows from the TF reciprocal relation $N_{bcc}(s) = s^{-3/2} N_{fcc}(1/s)$. Thus as t approaches infinity, $H(t)$ approaches $-\Delta X^{WS}$ from above. Since $H(\infty) = -\Delta X^{WS}$ and $H(\infty) > 0$, it follows *without numerical evaluation* from the order relations that ΔX^{WS} is negative for any *a-b* system obeying the same order relations as obeyed by the bcc-fcc system.

As t increases from zero ΔX starts out equal to the negative quantity ΔX^{WS}, increases to a maximum at $t = 1$ where it is positive, and then decreases to zero at infinity. This is verified with the numerical calculations discussed in Ref. 2 and shown here in Fig. 1. With additional information about how $\Delta N(s)$ varies in the domain $1 \leqslant s < \infty$, one can secure qualitative information about the relative sizes of $\Delta X(1)$ and ΔX^{WS}. Toward this end, use the reciprocity relation on the $N(s)$ and the defining expressions to rewrite ΔX^{WS} and $\Delta X(1)$ in the respective forms

$$\Delta X^{WS} = -\int_1^\infty \left(1 - \frac{1}{\sqrt{s}}\right) \Delta N(s)\, ds, \tag{22}$$

$$X(1) = \int_1^\infty \frac{1}{\sqrt{s}} \Delta N(s)\, ds. \tag{23}$$

Both integrands are non-negative over the whole domain of integration, and they are equal at $s = 4$. For the bcc-fcc system $\Delta N(s)$ has a maximum very close to $t = 1$ and is very nearly zero from about $s = 2$ to infinity. Thus $\Delta N(s)$ is appreciable where the integrand of Eq. (23) is larger than the integrand of Eq. (22), yielding for the bcc-fcc system $\Delta X(1) > |\Delta X^{WS}|$.

Equation (18) is convenient for evaluation of ΔX for t less than about 3/2. For larger t it is convenient to write $H(t) = -\Delta X^{WS} + \Delta X(t)$, which suggests writing

$$\Delta X(t) = -\int_0^{1/t} \Delta N(s)\, ds = \int_0^{1/t} \frac{\Delta N(1/s)}{s^{3/2}}\, ds = \int_t^\infty \frac{\Delta N(x)}{\sqrt{x}}\, dx, \tag{24}$$

which is readily evaluated.

To study ΔX for two lattices that are not mutually reciprocal one can return to Eqs. (13) and (14) to secure the appropriate modifications of Eqs. (17) and (18) as has been discussed for the fcc-sc and bcc-sc systems in Ref. 2. The positiveness of $H(t)$ for these two systems depends heavily on Eq. (19), and there are no zeros for ΔX. For the fcc-hcp system the role of Eq. (19) is replaced by[19]

$$N_{hcp}(s) > N_{fcc}(s), \quad 0 < s < \infty. \tag{25}$$

However, ΔN is much smaller for the fcc-hcp system than for the fcc-sc. Thus it is seen that certain qualitative information about TF's yields considerable information about the Madelung energy of the GWS.

III. THE FUCHS ENERGY

The Fuchs energy ϵ is independent of the particular summation cell (Sec. II) one uses except that, insofar as $K(\mathbf{r})$ enters, the same summation cells must be used everywhere. Let us use the same cells as those used for Eq. (7). Then the definition of the Fuchs energy is

$$\frac{2\epsilon}{Q^2} = \lim_{N\to\infty} \frac{1}{N}\left\{\sum_\tau^N \sum_{\tau'\neq\tau}^N \frac{1}{\Delta\tau} + \sum_\tau^N \sum_{\tau'}^N \left(\frac{p}{\pi}\right)^3 \int_0\int_0 \sum_w^\infty \sum_{w'}^\infty \frac{\exp[-p(\mathbf{z}-\mathbf{w})^2]\exp[-p(\mathbf{z}'-\mathbf{w}')^2]}{|\Delta\tau + \Delta\mathbf{z}|}\, d^3z d^3z' \right.$$
$$\left. - 2\sum_\tau^N \sum_{\tau'}^N \left(\frac{p}{\pi}\right)^{3/2} \int_0 \sum_w^\infty \frac{\exp[-p(\mathbf{z}-\mathbf{w})^2]}{|\Delta\tau + \mathbf{z}|}\, d^3z \right\}, \tag{26}$$

$$= \lim_{N\to\infty} \frac{1}{N}\left\{\sum_\tau^N \sum_{\tau'\neq\tau}^N \frac{1}{\Delta\tau} + \sum_\tau^N \sum_{\tau'}^N \frac{1}{\Omega^2} \int_0\int_0 \sum_\gamma^\infty \sum_{\gamma'}^\infty \frac{\exp[-(\gamma^2+\gamma'^2)/4p + i(\boldsymbol{\gamma}\cdot\mathbf{z} + \boldsymbol{\gamma}'\cdot\mathbf{z}')]}{|\Delta\tau + \Delta\mathbf{z}|}\, d^3z\, d^3z' \right.$$
$$\left. - 2\sum_\tau^N \sum_{\tau'}^N \frac{1}{\Omega} \int_0 \sum_\gamma^\infty \frac{\exp[-(\gamma^2/4p) + i\boldsymbol{\gamma}\cdot\mathbf{z}]}{|\Delta\mathbf{z} + \mathbf{z}|}\, d^3z \right\}, \tag{27}$$

where $\mathbf{w}$ and $\mathbf{w}'$ are τ lattices. Setting p equal zero in Eq. (27) secures Eq. (6) of Ref. 12 for the WS. Next group together the terms given by $\tau' = \tau$ in Eq. (27) to give

$$\frac{2\epsilon}{Q^2} = \frac{1}{\Omega^2} \int_0\int_0 \sum_\gamma^\infty \sum_{\gamma'}^\infty \frac{\exp[-(\gamma^2+\gamma'^2)/4p + i(\boldsymbol{\gamma}\cdot\mathbf{z}')]}{\Delta z}\, d^3z\, d^3z' - \frac{2}{\Omega} \int_0 \sum_\gamma^\infty \frac{\exp[-(\gamma^2/4p) + i\boldsymbol{\gamma}\cdot\mathbf{z}]}{z}\, d^3z$$
$$+ \lim_{N\to\infty} \frac{1}{N} \sum_\tau \sum_{\tau'\neq\tau} \quad \text{(remaining terms)}. \tag{28}$$

The next step of changing the summation limit on the τ' summation to infinity has not been previously justified even for the special case of the WS. As pointed out in Ref. 12, this step is required to get to Ihm and Cohen's[14] starting point for their definition of ϵ, and it was used in Ref. 12 to pass from its Eq. (8) to (9). The problem here is *exactly* the same as for the WS case, because the only difficulty arises from the contribution in Eq. (28) given by $\boldsymbol{\gamma}' = \boldsymbol{\gamma}$ which is identical to that for the WS. Proof that this step is valid is given in the Appendix.

With this step justified, one can, with a change to summation over $\Delta\tau$, write the last term in Eq. (28) as

$$\sum_{\tau}'\left\{\frac{1}{\tau}+\frac{1}{\Omega^2}\int_0\sum_{\gamma}\sum_{\gamma'}\frac{\exp[-(\gamma^2+\gamma'^2)/4p+i(\gamma\cdot\mathbf{z}+\gamma\cdot\mathbf{z}')]}{|\tau+\Delta\mathbf{z}|}\,d^3z\,d^3z'-\frac{2}{\Omega}\int_0\sum_{\gamma}\frac{\exp[-(\gamma^2/4p)+i\gamma\cdot\mathbf{z}]}{|\tau+\mathbf{z}|}\,d^3z\right\}. \tag{29}$$

Putting this into Eq. (28) and regrouping the terms gives

$$\epsilon=\frac{1}{2}K-\frac{1}{2}\frac{Q^2}{\Omega}\int_0\sum_{\gamma}\exp\left[-\left(\frac{\gamma^2}{4p}\right)+i\gamma\cdot\mathbf{z}\right]d^3z-\frac{1}{2}\frac{1}{\Omega}\int_0\sum_{\gamma}K(\mathbf{z})\exp\left[-\left(\frac{\gamma^2}{4p}\right)+i\gamma\cdot\mathbf{z}\right]d^3z. \tag{30}$$

This may be simplified and shown independent of the average potential by substituting $K=S+A$ and $K(\mathbf{r})=S(\mathbf{r})+A$, which leads to cancellation of the contributions from the two terms containing A. Thus Eq. (30) holds with K replaced by S and $K(\mathbf{r})$ replaced by $S(\mathbf{r})$, giving

$$\epsilon=\frac{1}{2}S-\frac{1}{2}\sum_{\gamma}\exp\left(\frac{-\gamma^2}{4p}\right)\frac{1}{\Omega}\int_0 S(\mathbf{z})\exp(i\gamma\cdot\mathbf{z})\,d^3z-\frac{1}{2}Q^2\sum_{\gamma}\exp\left(\frac{-\gamma^2}{4p}\right)\frac{1}{\Omega}\int_0\frac{\exp(i\gamma\cdot\mathbf{z})}{z}\,d^3z. \tag{31}$$

The second term of this can be simplified by using Eq. (14) to give

$$\begin{aligned}\frac{1}{\Omega}\int_0 S(\mathbf{z})\exp(i\gamma\cdot\mathbf{z})\,d^3z&=\frac{1}{\Omega}\int_0 S^{\mathrm{ws}}(\mathbf{z})\exp(i\gamma\cdot\mathbf{z})\,d^3z-\frac{4\pi Q^2}{\Omega}\frac{\exp(-\gamma^2/4p)}{\gamma^2},\quad \gamma\neq 0,\\&=\frac{1}{\Omega}\int_0 S^{\mathrm{ws}}(\mathbf{z})\,d^3z,\quad \gamma=0.\end{aligned} \tag{32}$$

After substituting this into Eq. (31), note that the integral of $S^{\mathrm{ws}}(\mathbf{z})$ over the centered summation cell is equal to the negative of the integral of z^{-1} over the cell, which yields

$$\begin{aligned}\epsilon=\frac{1}{2}S+\frac{2\pi Q^2}{\Omega}\sum_{\gamma}'\frac{\exp[-2(\gamma^2/4p)]}{\gamma^2}&-\frac{1}{2}\sum_{\gamma}'\exp\left(\frac{-\gamma^2}{4p}\right)\frac{1}{\Omega}\int_0 S^{\mathrm{ws}}(\mathbf{z})\exp(i\gamma\cdot\mathbf{z})\,d^3z\\&-\frac{1}{2}Q^2\sum_{\gamma}'\exp\left(\frac{-\gamma^2}{4p}\right)\frac{1}{\Omega}\int_0\frac{\exp(i\gamma\cdot\mathbf{z})}{z}\,d^3z.\end{aligned} \tag{33}$$

For final simplification, use Eq. (12) with p set equal to zero and $\nu=1/4u$ to give

$$S^{\mathrm{ws}}(z)=\frac{4\pi Q^2}{\Omega}\int_0^{\infty}\sum_{\gamma}\exp[-\gamma^2u+i\gamma\cdot\mathbf{z}]du-Q^2/z, \tag{34}$$

which with Eq. (33) yields

$$2\epsilon=S+\frac{4\pi Q^2}{\Omega}\sum_{\gamma}'\frac{[\exp(-\gamma^2/2p)-\exp(-\gamma^2/4p)]}{\gamma^2}, \tag{35}$$

and by Eq. (14)

$$\begin{aligned}2\epsilon=S^{\mathrm{ws}}-\frac{8\pi Q^2}{\Omega}\sum_{\gamma}'\frac{\exp[-\gamma^2/4p]}{\gamma^2}&\\+\frac{4\pi Q^2}{\Omega}\sum_{\gamma}'\frac{\exp[-\gamma^2/2p]}{\gamma^2}.&\end{aligned} \tag{36}$$

This completes the reduction of the definition of ϵ, involving a sequence of eighteen summations, to terms which involve only three summations which are readily evaluated.

IV. FUNCTIONAL RELATION BETWEEN ϵ AND S

A comparison of Eq. (14) for S with Eq. (36) for ϵ shows that a simple functional relation exists between the two. Let us first use it to show how to secure further expressions for ϵ and to verify that ϵ has the proper asymptotic form in the empty lattice limit.

For each of the five expressions of Eqs. (10)–(14) with r set equal to zero one can write a corresponding equation for ϵ by first relating ϵ and S through Eqs. (36) and (14) and then using a knowledge of how the second term in Eq. (14) contributes to the various terms in Eqs. (10)–(14) to determine what must be added to Eqs. (10)–(14) to secure a corresponding relation for 2ϵ. If this procedure is carried out for Eq. (11) with $r=0$, and if the first contribution for large p is considered as in Eqs. (15) and (16), one finds that Eq. (36) implies

$$2\epsilon\sim-2[2Q^2(p/\pi)^{1/2}]+2Q^2(p/2\pi)^{1/2}, \tag{37}$$

$$\epsilon\sim-(2-2^{-1/2})Q^2(p/\pi)^{1/2}. \tag{38}$$

This result is exactly what one can calculate directly from Eq. (26) as the leading contribution to ϵ for large p. Or, without reference to Eq. (26), note that as the local background near a point charge Q bunches up to become a point charge $-Q$, the leading term in ϵ is given by two terms: the interaction of the charge Q with the local Gaussian distribution and the interaction of the Gaussian with itself. These two are readily calculated and found to give Eq. (38). Though elementary in nature, this check on the accuracy of Eq. (36) is a stringent one.

For electrostatic structural transitions one wants to study the difference $\Delta\epsilon$ for two competing lattices. It is convenient to compare the reduced X and Y, where again $S=FX$ and $2\epsilon=FY$ with $F=Q^2/\Omega^{1/3}$, with $t=p(\Omega^{2/3}/\pi)$, and with Δ referring to a value on an a lattice minus the value of a b lattice, where for our first case the (a,b) forms a mutually-reciprocal unit lattice. Then

$$\begin{aligned}\Delta Y&=\Delta X+H(t)-H(t/2)\\&=\Delta X^{\mathrm{ws}}+2H(t)-H(t/2),\end{aligned} \tag{39}$$

with $H(t)$ given by Eqs. (17) and (18). Figure 1, taken from Ref. 2, shows how ΔY varies with t for the bcc-fcc system. Minor modifications are required for cases where the two lattices are not mutually reciprocal. The fcc-sc and bcc-sc systems are disussed in Ref. 2, and the fcc-hcp system where one lattice (hcp) is not Bravais has similar equations, but one should recall the discussion of Eq. (25). The sequence of lowest-energy structures with increasing t for the GWS is bcc, fcc, and sc, provided only the cubics are considered.[2]

Much can be determined about these transitions with no, or minimal, computations provided one has a modest amount of information about order relations on TF's for the lattices involved. I have discussed the role of the TF's in connection with S through the $H(t)$. The same considerations

apply to ϵ or Y, say through Eq. (39), and $H(t)$ and $H(t/2)$. It is the Gaussian function that leads to such an important role of the TF's in the GWS; in the YWS the role of TF's is less transparent. Nevertheless, there are a lot of similarities between the functional relation for the Y^{GWS} and X^{GWS} and that for the Y^{YWS} and X^{YWS} as shown in Ref. 2.

APPENDIX

Proving that one can pass from Eq. (28) to Eq. (29) reduces to the corresponding problem for the special case of the WS, because the only difficulty arises from the contribution to Eq. (27) given by $\gamma' = \gamma$. This task in turn reduces to that of proving $J = 0$, where

$$J = \lim_{N\to\infty} \frac{1}{N} \sum_{\tau}^{N} \sum_{\tau'>N}^{\infty} \left\{ \frac{1}{\Delta\tau} + \frac{1}{\Omega^2} \times \int_0\int_0 \frac{d^3z\, d^3z'}{|\Delta\tau + \mathbf{z}|} - \frac{2}{\Omega} \int_0 \frac{d^3z}{|\Delta\tau + \mathbf{z}|} \right\}. \tag{A1}$$

To prove that $J = 0$ note that

$$\frac{1}{|\mathbf{u}+\mathbf{w}|} = \frac{1}{u}\left\{1 - \frac{\mathbf{w}\cdot\hat{u}}{u} + \frac{1}{2u^2}\left[3(\mathbf{w}\cdot\hat{u})^2 - w^2\right]\right\} + O\left(\frac{1}{u^4}\right), \tag{A2}$$

which will be used with $\mathbf{u} = \Delta\tau$ and $\mathbf{w} = \Delta\mathbf{z}$ or $\mathbf{w} = \mathbf{z}$. Note further that for centered cells

$$\frac{1}{\Omega^2}\int_0\int_0 (\Delta z)^2\, d^3z\, d^3z' = \frac{2}{\Omega}\int_0 z^2 d^3z, \tag{A3}$$

$$\frac{1}{\Omega^2}\int_0\int_0 (\Delta\mathbf{z}\cdot\Delta\tau)^2\, d^3z\, d^3z' = \frac{2}{\Omega}\int_0 (\mathbf{z}\cdot\Delta\tau)^2\, d^3z\, d^3z'. \tag{A4}$$

Substitution of Eqs. (A2)–(A4) into Eq. (A1) gives

$$J = \lim_{N\to\infty} \frac{1}{N} \sum_{\tau} \sum_{\tau'>N}^{\infty} O\left[\frac{1}{(\Delta\tau)^4}\right], \tag{A5}$$

which is equal to zero.

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The Peierls–Griffiths argument for disordered Ising systems

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(Received 13 April 1981; accepted for publication 5 June 1981)

We study Ising systems with random competing ferromagnetic and antiferromagnetic nearest neighbor interaction on a simple cubic lattice of arbitrary dimension. We use a version of the Peierls–Griffiths argument to prove the existence of a ferromagnetic phase and derive lower bounds for the critical concentration of antiferromagnetic bonds.

PACS numbers: 75.10.Hk

I. INTRODUCTION

In a previous paper,[1] Avron, Schulman, and the author found a number of rigorous results for the Ising spin glass model. For reasons that will become apparent in a moment, the proofs were formulated for the two-dimensional case only, though the main interest is in the three-dimensional model. It was shown that a version of the Peierls–Griffiths argument[2,3] can be used to prove the existence of a ferromagnetic phase at sufficiently low temperature and for a small but nonzero concentration of antiferromagnetic bonds. By appeal to geometric intuition and introducing certain pictures, like g^* strings and r^* strings, we made the physics behind our proof more transparent. The basic philosophy then was that spin glasses are systems with "random geometry."

The purpose of the present paper is to go beyond $d = 2$ and to study in a systematic way some geometric properties of the Ising spin glass. The focus now is on the coboundary operator δ which is no doubt conceptually simple but somewhat less familiar to physicists. Not only does this notion allow us to formulate the Peierls–Griffiths argument in a much more general setting, but it also shows that the Ising spin glass may be viewed as a discrete version of Maxwell's theory with the exterior derivative replaced by δ and where the gauge group is $\mathbb{Z}_2$. We prove the existence of a ferromagnetic phase for the quenched system with nearest neighbor interaction. Using known techniques from random walk[4] we also improve the lower bound obtained in Ref. 1 for the critical concentration of antiferromagnetic bonds. The question whether there exists a genuine spin glass phase with nonzero Edwards–Anderson order parameter[5] in sufficiently high dimensions remains undecided. On the other hand, it is known[6] that the spherical model with long range interactions has a ferromagnetic as well as a spin glass phase.

2. PEIERLS CONTOUR IN ISING LATTICES

We consider the Ising model with underlying lattice $\mathbb{Z}^d$. For each finite $\Lambda \subset \mathbb{Z}^d$ we have the space $C^0(\Lambda) = \mathbb{Z}_2^\Lambda$ of configurations in Λ. One may either adopt the spin language and write $\mathbb{Z}_2 = \{+1, -1\}$ or use the lattice gas formulation and write $\mathbb{Z}_2 = \{0,1\}$. The latter version seems preferable since, mathematically speaking, $\{0,1\}$ is the prime number field of characteristic 2 which gives $C^0(\Lambda)$ the structure of a $\mathbb{Z}_2$-linear space with respect to pointwise addition of functions $a:\Lambda \to \{0,1\}$. The set of negative spins, $|a| = a^{-1}(1)$, is called the *support* of the function $a \in C^0(\Lambda)$. This then establishes a 1:1 correspondence between vectors in $C^0(\Lambda)$ and subsets of Λ. To the addition of vectors there corresponds the symmetric difference of their supports:

$$|a + b| = |a| \Delta |b|. \tag{2.1}$$

Note also that $a + a = 0$ which reflects the identity $1 + 1 = 0$ in $\mathbb{Z}_2$. Moreover, it is easy to see that the introduction of the norm

$$\|a\| = \operatorname{card}|a| \tag{2.2}$$

turns $C^0(\Lambda)$ into a normed vector space.

When dealing with nearest-neighbor interaction, we need to consider the set of bonds $B(\Lambda)$. At this point there is a certain amount of freedom: we may or may not include bonds that connect Λ to its complement in $\mathbb{Z}^d$. This has to do with the choice of boundary conditions. In the present paper we use positive boundary conditions (the "natural" ones for a lattice gas). Therefore, $B(\Lambda)$ is taken to be the set of all bonds having at least one bounding site in Λ. Any spin outside of Λ has value $+1$.

Suppose the interaction is ferromagnetic. Then we would say that a bond is satisfied (dissatisfied) in a configuration $a \in C^0(\Lambda)$ if the product of the spin variables at the two bounding sites is positive (negative). In geometric terms, the dissatisfied bonds connect the set $|a|$ to its complement. It is common practice to visualize the situation by associating, to each dissatisfied bond k, the $(d-1)$-dimensional orthogonal cell k^* of the dual lattice. The collection of k^*'s then forms a close hypersurface which can always be decomposed into minimal polyhedra with no common $(d-1)$-dimensional faces. Any minimal polydedron on the dual lattice is called a Peierls contour.

It will prove necessary to rephrase this construction in an algebraic language.[7] Let us thus introduce the vector space $C^1(\Lambda)$ of functions on the bonds $b:B(\Lambda) \to \{0,1\}$. There exists a linear map

$$\delta: C^0(\Lambda) \to C^1(\Lambda) \tag{2.3}$$

called the coboundary operator with the following interpretation. For any configuration a $C^0(\Lambda)$, the coboundary δa assigns values 0 and 1 to satisfied and dissatisfied bonds, respectively. Thus, if $|\delta a|$ is the set of dissatisfied bonds, then the Hamiltonian of the ferromagnetic Ising model is

a) On Leave from the Institute of Theoretical Physics, RWTH Aachen, Germany. This work was supported in part by the Stiftung Volkswagenwerk.

 0022-2488/81/123002-04$01.00

$$H(a) = 2J\|\delta a\| \quad (J>0) \tag{2.4}$$

normalized such that $H(0) = 0$.

Coboundaries δa form a linear subspace $B^1(\Lambda)$ of $C^1(\Lambda)$ and the map (2.3) is injective ($\delta a = 0$ implies $a = 0$) since we adopted positive boundary conditions. In other words, the coboundary δa determines the spin configuration uniquely.

Two coboundaries δa and $\delta a'$s are said to be *disjoint* if their supports are disjoint. In this case,

$$\|\delta a + \delta a'\| = \|\delta a\| + \|\delta a'\|. \tag{2.5}$$

A coboundary $\delta c \in B^1(\Lambda)$ is said to be a *Peierls contour* if it cannot be represented as a sum of disjoint coboundaries and if $\delta c \neq 0$. Consequently, any coboundary may be written as a sum of disjoint Peierls contours,

$$\delta a = \delta c_1 + \delta c_2 + \cdots + \delta c_n. \tag{2.6}$$

The geometric picture behind this construction suggests that the representation is in fact unique. A formal proof, however, requires a little algebraic topology and is omitted here since the uniqueness is immaterial for the Peierls–Griffiths argument.

In essence, the spin configuration is fixed by its Peierls contours, each contour δc contributing $2J\|\delta c\|$ to the energy (2.4). Notice also that $|c|$ is the set of sites inside the polyhedron associated with δc. Therefore, $\|c\|$ and $\|\delta c\|$ are measures of the volume and the surface of the polyhedron.

3. LARGE CONTOURS ARE UNLIKELY

We want to show that, for a certain class of Hamiltonians $H(a)$, a large contour δc is rather unlikely in the Gibbs state at low temperatures. The first step is to define the characteristic function

$$\chi_{\delta c}(a) = \begin{cases} 1 & |\delta c| \subset |\delta a|, \\ 0 & |\delta c| \not\subset |\delta a|. \end{cases} \tag{3.1}$$

The problem then is to estimate the probability

$$\langle \chi_{\delta c} \rangle_\Lambda = Z_\Lambda^{-1} \sum_a \chi_{\delta c}(a) e^{-\beta H(a)}, \tag{3.2}$$

where $\beta = 1/kT$ and

$$Z_\Lambda = \sum_a e^{-\beta H(a)}. \tag{3.3}$$

We assume that $H(a)$has been normalized such that $H(0) = 0$.

Theorem 1: Let the Hamiltonian $H(a)$ be such that $|\delta a| \cap |\delta a'| = \emptyset$ implies

$$H(a + a') \geqslant H(a) + H(a'). \tag{3.4}$$

Then

$$\langle \chi_{\delta c} \rangle_\Lambda \leqslant (1 + e^{\beta H(c)})^{-1}. \tag{3.5}$$

The hypothesis of this theorem expresses that the energy cannot become smaller when spin configurations are superposed provided their coboundaries are disjoint. It is characteristic of nearest-neighbor models that equality holds in (3.4). The theorem demonstrates that δc has small probability if $\beta H(c)$ is large.

Proof: We put $b = a + c$ so that $a = b + c$. If δc is a contour and if $a \in C^0(\Lambda)$ contributes to the sum (3.2), then $|\delta c| \cap |\delta b| = \emptyset$ and $H(a) \geqslant H(b) + H(c)$ by assumption. Therefore

$$Z_\Lambda \langle \chi_{\delta c} \rangle_\Lambda \leqslant e^{-\beta H(c)} \sum{}' e^{-\beta H(a)}, \tag{3.6}$$

where we changed the summation variable from b *to* a. The prime indicates that the summation is restricted by the condition $|\delta a| \cap |\delta c| = \emptyset$. This implies $|\delta a| \not\supset |\delta c|$ and hence

$$\sum{}' e^{-\beta H(a)} \leqslant Z_\Lambda \langle 1 - \chi_{\delta c} \rangle_\Lambda \tag{3.7}$$

which proves the theorem.

4. DISORDER AND FRUSTRATION

The simplest model of a spin glass has coupling constants $\pm J$ with random sign at each bond. Equivalently, we pick $b \in C^1(\Lambda)$ at random and write for the energy

$$H_b(a) = 2J(\|\delta a + b\| - \|b\|) \quad (J>0). \tag{4.1}$$

The interpretation is immediate: $|b|$ is the set of antiferromagnetic bonds and $|\delta a + b|$ is the set of bonds dissatisfied with respect to the event b. The term $-\|b\|$ in (4.1) is there merely to normalize the energy. We also assume that the coupling constants at different bonds are statistically independent and identically distributed. This amounts to giving the random variable b the probability distribution

$$p(b) = \text{const}\,[x/(1-x)]^{\|b\|} \quad (0<x<1), \tag{4.2}$$

where x is the concentration of antiferromagnetic bonds. The partition function

$$Z_\Lambda(b) = \sum_a \exp[-\beta H_b(a)] \tag{4.3}$$

is invariant under gauge transformations,[8] $b \to b + \delta a$. If b is a coboundary, the disorder can be eliminated from the system by a gauge transformation, and thus,

$$Z_\Lambda(\delta a) = Z_\Lambda(0). \tag{4.4}$$

Such events are said to have *irrelevant disorder*. To find a measure for relevant disorder[9] we introduce yet another space. This is the vector space $C^2(\Lambda)$ of functions $c: P(\Lambda) \to \{0,1\}$ where $P(\Lambda)$ is the set of plaquettes having at least one bounding face in $B(\Lambda)$. There exists a linear map $\delta: C^1(\Lambda) \to C^2(\Lambda)$ extending the coboundary operator such that $\delta^2 = 0$. For any $b \in C^1$, δb assigns the value 1 precisely to the frustrated plaquettes. Recall that a plaquette is said to be frustrated if an odd number of its bounding faces is antiferromagnetic. We call

$$f = \delta b \tag{4.5}$$

the *frustration* of the event b. The possible frustrations constitute a subspace B^2 of C^2. It is a proper subspace if $d \geqslant 3$. To find the condition that restricts the frustration pattern, we must take full advantage of the cochain complex[7]

$$0 \xrightarrow{\delta} C^1(\Lambda) \xrightarrow{\delta} C^2(\Lambda) \xrightarrow{\delta} C^3(\Lambda) \to \cdots, \tag{4.6}$$

where $\delta^2 = 0$. Let Z^n and B^{n+1} be the kernel and the image of the map $\delta: C^n \to C^{n+1}$. Then $B^n \subset Z^n$ and the quotient $H^n = Z^n/B^n$ is called the nth mod 2 cohomology space of Λ. The nth connectivity number $c_n = \dim H^n$ is an impor-

tant invariant of Λ. If $c_n = 0, 0 < n < d$, we would say that Λ has trivial topology. Let us examine two special cases.

(1) $c_1 = 0$, *hence* $B^1 = Z^1$. Since the partition function (4.3) merely depends on the orbit of b in C^1 under the gauge group B^1, it may be considered a function on $C^1/B^1 = C^1/Z^1 \cong B^2$. In other words, the partition function depends on the frustration f only and the equation $f = 0$ is a criterion for irrelevant disorder.

(2) $c_2 = 0$, *hence* $B^2 = Z^2$. The frustration satisfies the equation $f = 0$ which by assumption characterizes all possible frustration patterns. This equation says that flux tubes connecting frustrated plaquettes are always closed.

It is obvious that b and f resemble the potential and the field strength in Maxwell's theory. Typically, in lattices with trivial topology, f is observable and b is not.

5. FERROMAGNETISM IN DISORDERED SYSTEMS

The number of negative spins in a configuration $a \in C^0(\Lambda)$ is $N_-(a) = \|a\|$. We write

$$a = \sum \chi_{\delta c}(a) c, \tag{5.1}$$

where the sum is over all Peierls contours δc. The triangle inequality gives

$$N_-(a) \leqslant \sum \chi_{\delta c}(a) \|a\|. \tag{5.2}$$

Let $\langle \cdot \rangle_\Lambda(b)$ denote the thermal average with respect to the Hamiltonian (4.1) and $E(\cdot)$ denote the expectation with respect to the distribution (4.2). Then

$$E(\langle N_- \rangle_\Lambda) \leqslant \sum E(\langle \chi_{\delta c} \rangle_\Lambda) \|c\|. \tag{5.3}$$

A routine calculation shows that

$$H_b(a + a') = H_b(a) + H_b(a') \tag{5.4}$$

provided δa and $\delta a'$ are disjoint. By Theorem 1,

$$\langle \chi_{\delta c} \rangle_\Lambda(b) \leqslant (1 + \exp \beta H_b(c))^{-1}. \tag{5.5}$$

Moreover, $H_b(c) = 2J(n - 2k)$ where $n = \|\delta c\|$ and $k = \|\delta c| \cap |b\|$. The event that k out of n bonds are antiferromagnetic has probability $\binom{n}{k} x^k (1-x)^{n-k}$, and thus,

$$E(\langle \chi_{\delta c} \rangle_\Lambda) \leqslant \sum_k \binom{n}{k} \frac{x^k (1-x)^{n-k}}{1 + e^{2\beta J(n-2k)}}. \tag{5.6}$$

Similar estimates for random spin systems were derived by Griffiths and Lebowitz.[10] Using the formula

$$\pi^{-1} \int_0^\pi dt\, (2 \cos t)^n \cos(n - 2k)t = \begin{cases} \binom{n}{k} & 0 \leqslant k \leqslant n, \\ 0 & \text{otherwise,} \end{cases} \tag{5.7}$$

and the abbreviations $r = 2[x(1-x)]^{1/2}$, $p = x/(1-x)$, $q = 4\beta J$, we obtain

$$E(\langle \chi_{\delta c} \rangle_\Lambda) \leqslant \pi^{-1} \int_0^\pi dt\, f(t)\, (r \cos t)^{\|\delta c\|}, \tag{5.8}$$

where

$$f(t) = \sum_{m=-\infty}^{\infty} p^m (1 + e^{-mq})^{-1} \cos 2mt \tag{5.9}$$

($2m = n - 2k$ is even) assuming $0 < p < 1 < pe^q$. Clearly $\|\delta c\| = 2n_1 + 2n_2 + \cdots + 2n_d$ ($n_i \geqslant 1$) if $2n_i$ bonds of $|\delta c|$ run paralled to the ith axis. The idea is now to estimate the number $\Sigma' \|c\|$ where the the sum is over all Peierls contour δc with prescribed $n_1, \cdots, n_d$. Ruelle[11] proved

$$\sum{}' \|c\| \leqslant |\Lambda| \prod_{i=1}^{d} n_i^{1/(d-1)} 3^{2n_i - 1}. \tag{5.10}$$

From (5.3), (5.8), and (5.10),

$$|\Lambda|^{-1} E(\langle N_- \rangle_\Lambda) \leqslant I_d(x,T), \tag{5.11}$$

where

$$I_d(x,T) = \pi^{-1} \int_o^\pi dt\, f(t)\, g(t)^d \tag{5.12}$$

and

$$3g(t) = \sum_{n=1}^{\infty} n^{1/(d-1)} (3r \cos t)^{2n}. \tag{5.13}$$

The series converges if $x(1-x) < \frac{1}{36}$ hence $3r < 1$. Spontaneous magnetization occurs if the density of negative spins is less than $\frac{1}{2}$. In fact, (5.11) estimates this density independent of the size of the system. We have thus proved:

Theorem 2: For $x > 0$ and $T > 0$, both sufficiently small, the disordered Ising model is ferromagnetic if $d \geqslant 2$. A lower bound for the critical curve in the (x,T) plane is given by the equation $I_d(x,T) = \frac{1}{2}$.

At zero temperature, the function $f(t)$ assumes a particular simple form:

$$f(t) = (\tfrac{1}{2} - x)(1 - r^2 \cos^2 t)^{-1}. \tag{5.14}$$

Likewise, the function $g(t)$ looks simple if $d = 2$:

$$3g(t) = [(3r \cos t)^{-1} - 3r \cos t]^{-2}. \tag{5.15}$$

Numerical integration of (5.12) shows that the equation $I_2(x,0) = \frac{1}{2}$ is solved by $x = 0.01938\cdots$. As we increase the dimension, the critical values for x become slightly larger but never exceed 0.029 as given by the singularity at $3r = 1$. The constant 3 originates from our assertion that log 3 be the entropy per unit surface of the Peierls contour which is an overestimate.[12]

6. AN IMPROVED ESTIMATE

The numerical estimate for the average number of negative spins can be improved in one simple case: the two-dimensional spin glass at zero temperature. The previous argument uses an upper bound for the number of Peierls contours which is too generous for two reasons. (1) We counted open as well as closed contours and (2), we counted contours that intersect themselves. In two dimensions, the appropriate theory would be self-avoiding random walk. Still, useful results are scarce and highly nontrivial.

We carry the above analysis further by counting all closed paths that visit the dual sites in $\Lambda \subset \mathbb{Z}^2$, thereby obtaining an upper bond, independent of Λ, for the generating function ($r > 0$),

$$h_\Lambda(r) = |\Lambda|^{-1} \sum \|c\| r^{\|\delta c\|}, \tag{6.1}$$

where the sum is over Peierls contours δc. In fact, such an estimate is all we need to derive results for $T = 0$, because

$$|\Lambda|^{-1}E(\langle N_-\rangle_\Lambda)\leqslant\pi^{-1}\int_0^\pi dt\, f(t)h_\Lambda(r\cos t)$$
$$\leqslant\tfrac{1}{2}h_\Lambda(r) \tag{6.2}$$

as follows from (5.3), (5.8), and (5.14).

A closed path visiting dual sites has an even number of $\pi/2$ turns called vertices. Let $2k$ be this number. We single out a vertex and walk around: n steps along the x axis, n' steps along the y axis, and so on. Thus, closed paths are mapped onto $0\neq n_i,n_i'\in\mathbb{Z}$, $1\leqslant i\leqslant k$ $(k\geqslant 2)$ where $\Sigma n_i=\Sigma n_i'=0$ which is the closure condition. Let C_n^k be the number of ways one can choose integers $n_1,\ldots,n_k$ such that $n_i\neq 0$, $\Sigma n_i=0$, and $\Sigma|n_i|=2n$. The generating function

$$F_k(r)=\sum_{n=k}^{\infty}C_n^k r^{2n}\quad(0\leqslant r<1) \tag{6.3}$$

may be represented as

$$F_k(r)=(2\pi)^{-1}\int_{-\pi}^{\pi}ds\,(P_r(s)-1)^k, \tag{6.4}$$

where $P_r(s)$ is the Poisson kernel,

$$P_r(s)=\sum_{n=-\infty}^{\infty}r^{|n|}e^{ins}=\mathrm{Re}\,\frac{e^{is}+r}{e^{is}-r}. \tag{6.5}$$

The number of loops in Λ with $2k$ vertices and total length $2n+2n'$ is certainly smaller than $|\Lambda|(2k)^{-1}C_n^k C_{n'}^k$. The factor $|\Lambda|$ arises from the fact that translated loops have to be distinguished. We also divided by $2k$ since the walk on the dual lattice may be started at any of the $2k$ vertices. The area enclosed by the loop may be bounded as $\|c\|\leqslant n\,n'$. This gives $h_\Lambda(r)\leqslant Q(r)$ where

$$Q(r)=\sum_{k=2}^{\infty}\Big(\sum_{n=k}^{\infty}nC_n^k r^{2n}\Big)^2(2k)^{-1}$$
$$=\sum_{k=2}^{\infty}\Big(\frac{r}{2}\frac{d}{dr}F_k(r)\Big)^2(2k)^{-1}. \tag{6.6}$$

The sum is convergent provided $3r<1$. From (6.4),

$$2Q(r)=\pi^{-2}\int_0^\pi ds\int_0^\pi ds'\,A(s,s')\,C(s)\,C(s'), \tag{6.7}$$

where $A=(1-B)^{-2}-1$ and

$$B(s,s')=(P_r(s)-1)(P_r(s')-1), \tag{6.8}$$
$$C(s)=\mathrm{Re}\,re^{is}(e^{is}-r)^{-2}. \tag{6.9}$$

We may replace A by $A+1$ in (6.7) without changing the integral. Moreover, the integral with respect to s' can be performed analytically leaving

$$Q(r)=2\Big(\frac{r^2}{1-r^2}\Big)^2\frac{1}{\pi}\int_0^\pi ds\,\frac{[2r-(1+r^2)\cos s](r-\cos s)}{[(1+3r^2-2r\cos s)^2-4r^2]^{3/2}}. \tag{6.10}$$

which is nonsingular if $3r<1$. Note that $Q(r)$ may be written as a sum of three elliptic integrals. Using either this representation or numerical integration one shows that the critical value $Q(r)=1$ is assumed for r $=0.3319\cdots$corresponding to $x=0.02834\cdots$ since $r^2=4x(1-x)$. The result is considerable improvement over the previous lower bound for the critical concentration x_c of antiferromagnetic bonds in the two-dimensional spin glass at zero temperature.

ACKNOWLEDGMENTS

I would like to thank Joseph Avron, Lawrence Schulman, Joel Lebowitz, and Michael Aizenman for stimulating discussions.

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A null tetrad analysis of the Ernst metric

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(Received 22 December 1980; accepted for publication 24 July 1981)

The Ernst metric is analyzed in terms of the null tetrad formalism of Newman and Penrose. Some applications of the formalism are also given.

PACS numbers: 97.60.Lf

An exact electrovac solution of the Einstein–Maxwell field equations has been found by Ernst,[1] which could provide a model for the exterior metric due to a Schwarzschild black hole embedded in a magnetic field. The Ernst solution, which is static, axially-symmetric, but not asymptotically flat, could hopefully yield a valid approximation to the realistic situation, at least in the near zone of a black hole. The geometry of the event horizon for this metric has recently been studied by Wild and Kerns.[2] In this note we carry out an analysis of the Ernst metric, in terms of the null tetrad formalism of Newman and Penrose.[3] We choose a system of null tetrads and calculate the spin coefficients and the tetrad projections of the various tensors of interest, e.g., the Weyl, the Ricci, and the electromagnetic field tensor. As an application of these results, we study the principal null vectors of the Weyl tensor. We find that the Ernst metric is algebraically general, of type I in the Petrov classification.

As another application, we derive an expression for the Gaussian curvature of the event horizon and thereby reproduce the result of Ref. 2. As a final application, we derive the form of the electromagnetic test fields. We find that nontrivial test fields do not exist.

We shall consider a tetrad of null vectors $\{l_\mu, n_\mu, m_\mu, m_\mu^*\}$ satisfying the usual conditions

$$l_\mu n^\mu = -m_\mu m^{*\mu} = 1, \quad l_\mu m^\mu = n_\mu m^\mu = 0, \tag{1}$$

$$g_{\mu\nu} = l_\mu n_\nu + n_\mu l_\nu - m_\mu m_\nu^* - m_\mu^* m_\nu. \tag{2}$$

In a Schwarzschild-like coordinate system with $x^0 = t$, $x^1 = r$, $x^2 = \theta$, and $x^3 = \phi$ the Ernst solution has the line element

$$ds^2 = g_{\mu\nu}dx^\mu dx^\nu = \Lambda^2[(1-2m/r)dt^2 - (1-2m/r)^{-1}dr^2 - r^2 d\theta^2] - \Lambda^{-2} r^2 \sin^2\theta\, d\phi^2, \tag{3}$$

where

$$\Lambda = 1 + \tfrac{1}{4}B^2 r^2 \sin^2\theta \tag{3a}$$

and B is the parameter of the (external) magnetic field, whose Cartan components are

$$H_r = \Lambda^{-2} B\cos\theta, \quad H_\theta = -\Lambda^{-2} B(1-2m/r)^{1/2}\sin\theta. \tag{3b}$$

Then the following choice of the null tetrad

$$l_\mu = (1, -(1-2m/r)^{-1}, 0, 0),$$
$$n_\mu = (\Lambda^2/2)(1-2m/r, 1, 0, 0),$$
$$m_\mu = \frac{r}{\sqrt{2}}\left(0, 0, -\Lambda, \frac{-i\sin\theta}{\Lambda}\right) \tag{4}$$

is easily shown to yield the Ernst metric via Eq. (2). With the tetrad now chosen [as in Eq. (4)], it is now a matter of straightforward calculation to compute the twelve spin coefficients. We find the following expressions:

$$\kappa = 0, \quad \nu = 0, \quad \epsilon = 0,$$
$$\sigma = -\frac{2}{r\Lambda^3}(\Lambda - 1), \quad \lambda = -\frac{\Lambda - 1}{r\Lambda}\left(1 - \frac{2m}{r}\right),$$
$$\rho = -\frac{1}{r\Lambda^2}, \quad \alpha = -\frac{\cot\theta}{2(\sqrt{2})r\Lambda}, \tag{5}$$
$$\beta = \frac{\cot\theta}{2(\sqrt{2})r\Lambda^2}(4 - 3\Lambda), \quad \tau = \alpha + \beta, \quad \pi = -\tau,$$
$$\mu = -\frac{1}{2r}\left(1 - \frac{2m}{r}\right), \quad \gamma = \frac{m}{2r^2} + \frac{\Lambda - 1}{r\Lambda}\left(1 - \frac{2m}{r}\right),$$

where the notation for the spin coefficients is the same as in Ref. 3. From the above expressions we can now calculate the tetrad projections of the Weyl and the Ricci tensors by use of the Newman–Penrose equations. For instance, the equation

$$D\sigma - \delta\kappa = \sigma(\rho + \rho^* + 3\epsilon - \epsilon^*) - \kappa(\tau - \pi^* + \alpha^* + 3\beta) + \Psi_0 \tag{6}$$

gives the Weyl tensor component ψ_0. Thus using eleven of the eighteen Newman–Penrose equations we find

$$\Psi_0 = \frac{6(\Lambda - 1)(\Lambda - 2)}{r^2\Lambda^6}, \quad \Psi_1 = \frac{\Lambda\cot\theta}{\sqrt{2}}\Psi_0,$$
$$\Psi_3 = -(\Lambda^2/2)\left(1 - \frac{2m}{r}\right)\Psi_1, \quad \Psi_4 = (\Lambda^4/4)\left(1 - \frac{2m}{r}\right)^2\Psi_0, \tag{7}$$
$$\Psi_2 = \frac{\Lambda - 2}{r^2\Lambda^4}\left[(2\cot^2\theta - 1)(\Lambda - 1) + \frac{m}{r}(3\Lambda - 2)\right].$$

The tetrad projections of the Ricci tensor are given by

$$\Phi_{ij} = 2\Phi_i\Phi_j^*, \quad i,j = 0,1,2, \tag{8}$$

where the tetrad projections of the electromagnetic field tensor are as follows:

$$\Phi_0 = \frac{i\sin\theta}{2^{1/2}\Lambda^3}B, \Phi_1 = (\Lambda/2^{1/2})\cot\theta\Phi_0,$$
$$\Phi_2 = -(\Lambda^2/2)(1 - 2m/r)\Phi_0. \tag{9}$$

We have used the standard notation[3] in writing Eqs. (6)–(9), above.

The Weyl and the electromagnetic tensor can be given a more symmetrical appearance by applying the null tetrad rotation

$$l'_\mu = \frac{1}{A}l_\mu, \quad n'_\mu = An_\mu, \quad m'_\mu = m_\mu \tag{10}$$

with

$$A = (2^{1/2}/\Lambda)(1 - 2m/r)^{-1/2}. \tag{10a}$$

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As a result, the Weyl tensor acquires the shape

$$\Psi_0' = \Psi_4' = \frac{3(\Lambda-1)(\Lambda-2)}{r^2\Lambda^4}\left(1-\frac{2m}{r}\right),$$
$$\Psi_1' = -\Psi_3' = \cot\theta\,(1-2m/r)^{-1/2}\Psi_0', \quad \Psi_2' = \Psi_2, \tag{11}$$

and the E.M. (electromagnetic) tensor becomes

$$\Phi_0' = -\Phi_2' = \frac{iB}{2\Lambda^2}\sin\theta\left(1-\frac{2m}{r}\right)^{1/2}, \quad \Phi_1' = \Phi_1, \tag{12}$$

where we have denoted by a superior prime quantities evaluated with respect to the tetrad system of Eqs. (10) and (10a). Similarly, the transformed spin coefficients are given by

$$\kappa' = 0, \quad \nu' = 0, \quad \sigma' = \sigma/A, \quad \rho' = \rho/A,$$
$$\lambda' = A\lambda, \quad \mu' = A\mu, \quad \tau' = \tau, \quad \pi' = -\tau', \tag{13}$$
$$\gamma' = (A/2)\gamma, \quad \epsilon' = \gamma', \quad \alpha' = -[(\Lambda-2)/\Lambda]\alpha, \quad \beta' = -\alpha'.$$

We make a few remarks on the tetrad systems given by Eqs. (4) and (10). The vectors l_μ and l'_μ each form a congruence of null geodesics. The geodesics corresponding to the l_μ vectors are affinely parametrized ($\epsilon = 0$) and the congruence of the vectors is equal to a gradient field ($\alpha + \beta = \tau$). The tetrad system of Eq. (4) reduces, in the limiting case of no magnetic field, to the Kinnersley's tetrad for the Schwarzschild metric. The null geodesic congruence formed by the l'_μ vectors is not affinely parametrized and one also notes that the expansion ρ' and the shear σ' of the l'_μ vectors vanish at the event horizon.

The expressions for the tetrad projections of the Weyl and the Maxwell tensors can be derived in a much more efficient manner (than via the use of the Newman–Penrose equations) by utilizing an elegant technique developed by Hauser and Ernst.[4] These authors have given compact expressions for these projections for *any* electrovac spacetime which results from a given seed solution of the Einstein–Maxwell equations when the seed solution is subjected to a transformation of the Kinnersley group. A derivation along these lines has been obtained by Ernst and is being quoted here with his permission.[5] The Weyl tensor is given by Eq. (5.9) of Ref. 4 and reads, in the notation of that paper, as

$$(C^{AB})' = \Lambda^{-2}(1-2b_E f\Lambda^{-1}) \times\{C^{AB} + 12b_E\Lambda^{-1}[\omega^A\omega^B - \tfrac{1}{3}(\omega^C\omega_C)G^{AB}]\}, \tag{14}$$

where C^{AB} is the Weyl tensor of the Schwarzschild solution which is the seed solution for the present case. The first step in calculating the remaining terms that appear in the above, is to select a Killing vector for the seed solution. This is taken to be $K^\mu\partial_\mu = \partial_\phi$ and from the concomitant one-form $K = r^2\sin^2\theta\,d\phi$ one next constructs the two-form

$$\omega = \tfrac{1}{2}dK = r\sin^2\theta\,dr\wedge d\phi + r^2\sin\theta\cos\theta\,d\theta\wedge d\phi. \tag{15}$$

The next step is to choose a convenient basis $\{B_A\}$ for the two-forms.

$$B_+ = k\wedge t, \quad B_0 = k\wedge m + t\wedge t^*, \quad B_- = m\wedge t^*, \tag{16}$$

where

$$k = (1/2^{1/2})((1-2m/r)^{-1/2}dr - (1-2m/r)^{1/2}dt),$$
$$m = (1/2^{1/2})((1-2m/r)^{-1/2}dr + (1-2m/r)^{1/2}dt), \tag{17}$$
$$t = (r/2^{1/2})(d\theta + i\sin\theta d\phi).$$

The null tetrad $\{k,m,t,t^*\}$ in the Hauser–Ernst notation corresponds to the null tetrad $\{l,n,m,m^*\}$ in the Newman–Penrose notation. Also, the different sign convention for the line element adopted by Hauser–Ernst, as compared to Newman–Penrose, should be noted.[6] The desired quantities that appear in Eq. (14) are then given by

$$\omega_A = B_A\lrcorner\omega, \quad G^{AB} = B^A\lrcorner B^B,$$
$$f = K\lrcorner K = -r^2\sin^2\theta, \tag{18}$$

where $\lrcorner$ denotes the inner product as defined in Ref. 4. In addition

$$b_E = -\tfrac{1}{4}B^2, \quad \Lambda = 1 + \tfrac{1}{4}B^2r^2\sin^2\theta \tag{19}$$

as follows directly from the relevant Kinnersley transformation. Putting together Eqs. (15)–(19) and remembering[6] the connection between the two notations

$$(C^{-1-1})' = -\Psi_0, \quad (C^{-10})' = -\Psi_1, \quad (C^{00})' = -\Psi_2,$$
$$(C^{11})' = -\Psi_4, \quad (C^{10})' = -\Psi_3, \tag{20}$$

we obtain from Eq. (14) the expressions for the Weyl tensor as given by Eq. (11). Similarly, Eq. (3.3) of Ref. 4 gives the electromagnetic field

$$(F_A)' = B\Lambda^{-2}\omega_A \tag{21}$$

which is our Eq. (12). We note that all the tetrad projections have nice behavior as $r\to\infty$.

We wish now to consider applications of the foregoing results. As a first application, we want to find the principal null vectors of the Weyl tensor. As explained by Janis and Newman,[7] this can be done by solving the quartic equation

$$\Psi_4 b^4 + 4\Psi_3 b^3 + 6\Psi_2 b^2 + 4\Psi_1 b + \Psi_0 = 0. \tag{22}$$

Now the coefficients of the above equation enjoy the property

$$\Psi_0/\Psi_4 = (\Psi_1/\Psi_3)^2, \tag{23}$$

as we can see from Eq. (7). Using (23), the quartic equation (22) may be replaced by a quadratic equation

$$\Psi_4 y^2 + 4\Psi_3 y + 6\Psi_2 - 2\Psi_4(\Psi_1/\Psi_3) = 0 \tag{24}$$

in terms of the variable

$$y = b + \Psi_1/\Psi_3 b. \tag{24a}$$

Thus the quartic equation (22) can be solved in two steps; each step involves solving a quadratic equation. The roots b_i ($i = 1,2,3,4$) of Eq. (22) are thus found to be

$$b_{1,2} = \tfrac{1}{2}y_1 \pm \tfrac{1}{2}[y_1^2 + (8/\Lambda^2)(1-2m/r)^{-1}]^{1/2},$$
$$b_{3,4} = \tfrac{1}{2}y_1^* \pm \tfrac{1}{2}[y_1^{*2} + (8/\Lambda^2)(1-2m/r)^{-1}]^{1/2}, \tag{25}$$

where

$$y_1 = \frac{2}{\Lambda}\left(1-\frac{2m}{r}\right)^{-1}\left[(2^{1/2})\cot\theta + i\left(\frac{m\Lambda}{r(\Lambda-1)}\right)^{1/2}\right] \tag{25a}$$

and y_1^* is the complex conjugate of y_1. Thus the Weyl tensor has four principal null vectors corresponding to the four distinct simple roots of Eq. (22). The metric, therefore, is algebraically general, of type I according to the Petrov classification. We also note that in the limit $m = 0$ of the Melvin metric,[8] we have $y_1 = y_1^*$ and Eq. (22) now has a pair of double roots. Thus the Melvin metric is of type D, as has been recently noted by Wild.[9]

As a second application, let us consider the Gaussian curvature of the event horizon. The expression for the Gaussian curvature in terms of the Newman–Penrose quantities was found by Hartle,[10] for vacuum metrics. Adapting his derivation to the electrovac case, we easily obtain the formula

$$\mathscr{R} = 4\,\mathrm{Re}(\rho\mu - \lambda\sigma - \Psi_2 + \Phi_{11}) \tag{26}$$

for the Gaussian curvature, as defined by Hartle.[10] Inserting the expressions for the spin coefficients from (5), ψ_2 from (7) and Φ_{11} from (8) and (9) and specializing to the horizon at $r = r_0 = 2m$ and simplifying, we obtain from (26)

$$\mathscr{R} = \frac{2}{r_0^2 \Lambda_0^4}\left[-\Lambda_0^2(1 + 4\cot^2\theta) + 2\Lambda_0(1 + 8\cot^2\theta) - 12\cot^2\theta\right], \tag{27}$$

where Λ_0 is Λ evaluated at $r = r_0$. In terms of the dimensionless parameter $\bar{\beta} = mB = (\Lambda_0 - 1)^{1/2}/\sin\theta$, Eq. (27) is easily rewritten as

$$\mathscr{R} = \frac{2}{r_0^2 \Lambda_0^4}\left[\Lambda_0^2 + 2\bar{\beta}^2\Lambda_0(4\cos^2\theta - \sin^2\theta) - 12\bar{\beta}^4\sin^2\theta\cos^2\theta\right], \tag{28}$$

which is exactly the expression derived in Ref. 2, using a different method (notice that Hartle's $\mathscr{R}$ is twice the Gaussian curvature as defined by Wild and Kerns).

As a final application, we will derive the form of the electromagnetic *test fields* on the Ernst metric. For this purpose it is convenient to choose a tetrad system in which two of the null vectors are chosen to be along the principal null vectors of the electromagnetic tensor, so that

$$\tilde{\Phi}_0 = 0, \quad \tilde{\Phi}_2 = 0, \tag{29}$$

where by an overtilde we mean that the relevent quantity is evaluated with respect to the new tetrad system. The desired tetrad rotations (two successive rotations) that lead to Eq. (29) are easily found and applying the standard formulas for tetrad rotations,[11] we thus obtain

$$\tilde{\Phi}_1 = -(iB/2\Lambda^2)\cos\theta\sqrt{R}, \tag{30}$$

$$\tilde{\rho} = \frac{3m}{r^2 R\Lambda^2}\frac{\tan^2\theta}{(1 - \sqrt{R})},$$

$$\tilde{\mu} = \frac{3m}{8r^2R^2}(R - 1)(1 - \sqrt{R}), \tag{30a}$$

$$\tilde{\pi} = -\tilde{\tau} = \frac{\tan\theta}{2(\sqrt{2})r\Lambda R^{3/2}} \times\left[\frac{m}{r}(R - 3) - 4\frac{\Lambda - 1}{\Lambda}R^2\cot^2\theta\right], \tag{30b}$$

where

$$R = 1 + (1 - 2m/r)\tan^2\theta. \tag{31}$$

The Newmann–Penrose operators are calculated similarly.

$$\tilde{D} = \frac{2}{\Lambda^2(R^{1/2} - 1)}\left[\frac{\sqrt{R}}{R - 1}\tan^2\theta\frac{\partial}{\partial t} - \frac{\partial}{\partial r} + \frac{\tan\theta}{r}\frac{\partial}{\partial\theta}\right],$$

$$\tilde{\Delta} = \frac{R^{1/2} - 1}{4R}(R - 1)\cot^2\theta \times\left[\frac{\sqrt{R}}{R - 1}\tan^2\theta\frac{\partial}{\partial t} + \frac{\partial}{\partial r} - \frac{\tan\theta}{r}\frac{\partial}{\partial\theta}\right], \tag{32}$$

$$\tilde{\delta} = -\frac{\cot\theta}{(\sqrt{2})\Lambda(\sqrt{R})}\left[(R - 1)\frac{\partial}{\partial r} + \frac{\tan\theta}{r}\frac{\partial}{\partial\theta}\right] + \frac{i\Lambda}{(\sqrt{2})r\sin\theta}\frac{\partial}{\partial\phi}.$$

Let us now introduce perturbation fields $\tilde{\Phi}_i^P$ and write the net electromagnetic field as $(\tilde{\Phi}_i + \tilde{\Phi}_i^P)$, where $\tilde{\Phi}_i$ is the unperturbed field. In the test field approximation, the background metric and hence the energy-momentum tensor is held fixed, and the condition for the vanishing of the first-order variation of the latter is

$$\tilde{\Phi}_i\tilde{\Phi}_j^{*P} + \tilde{\Phi}_j^*\tilde{\Phi}_i^P = 0. \tag{33}$$

Using (29) and the fact that $\tilde{\Phi}_1 \neq 0$, we obtain from the above

$$\tilde{\Phi}_0^P = \tilde{\Phi}_2^P = 0, \tag{34}$$

$$\tilde{\Phi}_1\tilde{\Phi}_1^{*P} + \tilde{\Phi}_1^*\tilde{\Phi}_1^P = 0. \tag{35}$$

The sourceless Maxwell's equations for the surviving test field now read

$$(\tilde{D} - 2\tilde{\rho})\tilde{\Phi}_1^P = (\tilde{\Delta} + 2\tilde{\mu})\tilde{\Phi}_1^P = 0,$$
$$(\tilde{\delta} - 2\tilde{\tau})\tilde{\Phi}_1^P = (\tilde{\delta}^* + 2\tilde{\pi})\tilde{\Phi}_1^P = 0. \tag{36}$$

From (30a), (30b), (32), and (36) it follows immediately that

$$\frac{\partial}{\partial t}\tilde{\Phi}_1^P = \frac{\partial}{\partial\phi}\tilde{\Phi}_1^P = 0 \tag{37}$$

and the resulting static, axisymmetric test field is then easily obtained from the remaining Maxwell's equations. We find thus

$$\tilde{\Phi}_1^P = (c/\Lambda^2)\cos\theta\sqrt{R}. \tag{38}$$

The infinitesimal parameter c must be real in order that (35) is satisfied. Since (38) can be obtained from (30) via a duality rotation, it is quite clear that the above perturbation corresponds to putting an (infinitesimal) external electric field around the source. In any event, nontrivial perturbations are ruled out in the test-field approximation. The situation here is exactly the same as in the case of the charged Kerr metric.[12]

ACKNOWLEDGMENT

It is a pleasure to thank Professor F. J. Ernst for his interest in the present work and for instructive correspondence.

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Addendum: Objects for the symmetric group [J. Math. Phys. 22, 1144 (1981)]

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(Received 25 September 1981; accepted for publication 1 October 1981)

PACS numbers: 02.20.Df

The programs which generate the results presented in this paper have now been published[1,2] and are obtainable as described in these references.

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ERRATA

Erratum: Algebraically special Yang-Mills solutions without sources [J. Math. Phys. 22, 2040 (1981)]

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(Received 13 January 1981; accepted for publication 6 March 1981)

PACS numbers: 11.10.Np, 99.10. + g

All the corrections occur in the Theorem and the Remark following it in Appendix C.

(1) In line (3) of the statement of the Theorem replace $H^2(M - \pi(\Sigma),R^*) = 0$ by $H^1(M - \pi(\Sigma),R^*) = 0$.

(2) In line (5) of the Remark replace 2-cocycle by 1-cocycle.

(3) In line (10) of the Remark replace 2-coboundary by 0-cocycle and add the statement: Every 0-cocycle b gives rise to a 1-coboundary c defined by $c_{UV} = b_U b_V^{-1}$.

(4) In line (11) of the Remark replace $H^2(M - \pi(\Sigma),R^*) = 0$ by $H^1(M - \pi(\Sigma),R^*) = 0$ and replace 2-cocycle by 1-cocycle.

(5) In line (12) of the Remark replace 2-coboundary by 0-cocycle.

Erratum: A kernel of Gel'fand–Levitan type for the three-dimensional Schrödinger equation [J. Math. Phys. Vol. 21, 83 (1980)]

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(Recieved 22 July 1981; accepted for publication 11 September 1981)

PACS numbers: 03.65.Nk, 99.10. + g

In Eqs. (38)–(40) the quantity $d\theta$ should be replaced by $\sin\theta\, d\theta$. That is, a factor $\sin\theta$ is missing. The equations which depend on Eqs. (38)–(40) are correct.

 0022-2488/81/123010-01$00.00