Matrices, differential operators, and polynomials

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It is noted that the matrix **Z**, of order n, defined in terms of the n arbitrary numbers x_j by the formula $Z_{jk} = \delta_{jk} \Sigma'_{l=1,n} (x_j - x_l)^{-1} + (1-\delta_{jk})(x_j - x_k)^{-1}$, may be considered (in an appropriate framework) to correspond to the differential operator d/dx. There follow prescriptions to construct explicit matrices of (arbitrary) order n in terms of n (or more) arbitrary numbers or of the n roots of given polynomials, matrices whose eigenvalues (and eigenvectors) are given, fully or in part, by very simple formulas. Novel representations of the classical polynomials (Hermite, Laguerre, Lagrange, Gegenbauer, Jacobi) are also obtained, such as the formula for Hermite polynomials $H_n(x) = 2^n \det[x\mathbf{I} - \mathbf{H}(\varphi)]$, where **I** is the unit matrix (of order n) and the matrix $\mathbf{H}(\varphi)$, of order n, is defined by $H_{jk}(\varphi) = (2n)^{-1/2}(\delta_{jk}(n-1)[\exp(2i\theta_j) + \frac{1}{2}\exp(-2i\theta_j)] + (1-\delta_{jk})\{-\exp(2i\theta_j) + [2i\sin(\theta_j - \theta_k)]^{-1}\exp[-i(\theta_j+\theta_k)]\})$, with $\theta_j = \varphi + \pi j/n$, φ arbitrary.

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I. INTRODUCTION

Certain remarkable properties of the zeros of the classical polynomials have been recently uncovered.[1-7] The prototype of these results is the statement[1,2] that the Hermitian matrix **A**, of order n, defined by

$$A_{jk} = \delta_{jk} \sum_{l=1}^{n}{}' (x_j - x_l)^{-2} - (1-\delta_{jk})(x_j - x_k)^{-2}, \tag{I.1}$$

has the first n nonnegative integers, $m = 0,1,...,n-1$, as eigenvalues, if the numbers x_j are the n zeros of the Hermite polynomial of order n,

$$H_n(x_j) = 0, \quad j = 1,2,...,n. \tag{I.2}$$

It has been, moreover, noted[3] that the (generally non-Hermitian) matrix **N**, of order n, defined by

$$N_{jk} = \delta_{jk} x_j \sum_{l=1}^{n}{}' (x_j - x_l)^{-1} + (1-\delta_{jk}) x_j (x_j - x_k)^{-1}, \tag{I.3}$$

also has the first n nonnegative integers as eigenvalues, but now for any arbitrary choice of the n numbers x_j (all different, of course). And a third typical result[3,6] states that the Hermitian matrix $\mathbf{L}(\theta)$, of order n, defined by

$$L_{jk}(\theta) = \delta_{jk} x_j \cos\theta + (1-\delta_{jk}) i(x_j - x_k)^{-1} \sin\theta, \tag{I.4}$$

has eigenvalues independent of θ, if the x_j's are again the n zeros of the Hermite polynomial of order n; see (I.2). Thus the eigenvalues of $\mathbf{L}(\theta)$ coincide with the x_j's themselves [since for $\theta = 0$, $L(\theta)$ is diagonal], and the following representation for Hermite polynomials holds:

$$H_n(x) = 2^n \det[x\mathbf{I} - \mathbf{L}(\theta)]. \tag{I.5}$$

This formula is trivial for $\theta = 0$, but not so for $\theta \neq 0$.

These results were originally obtained as by-products of the investigation of certain integrable dynamical systems.[2,8] Subsequently a more direct approach to their derivation, based on complex integration, was developed.[3] The main purpose of the investigation reported in this paper has been to cast these results in a more algebraic framework. In so doing, we have found many additional results of this kind. These include prescriptions to construct explicit matrices of (arbitrary) order n in terms of n (or more) arbitrary numbers or of the n roots of given polynomials, matrices whose eigenvalues (and eigenvectors) are given, fully or in part, by very simple formulas. Novel representations of the classical polynomials are also obtained, such as the formula for Hermite polynomials

$$H_n(x) = 2^n \det[x\mathbf{I} - \mathbf{H}(\varphi)], \tag{I.6}$$

with the matrix $\mathbf{H}(\varphi)$, of order n, defined by

$$H_{jk}(\varphi) = (2n)^{-1/2}(\delta_{jk}(n-1)[\exp(2i\theta_j) + \tfrac{1}{2}\exp(-2i\theta_j)] + (1-\delta_{jk})\{-\exp(2i\theta_j) + [2i\sin(\theta_j - \theta_k)]^{-1}\exp[-i(\theta_j+\theta_k)]\}), \tag{I.7}$$

where

$$\theta_j = \varphi + \pi j/n, \quad j = 1,2,...,n, \tag{I.8}$$

the quantity φ being arbitrary.

But perhaps more important than these specific findings is the connection that has emerged between the items mentioned in the title of this paper. Linear differential operators, matrices, and polynomials constitute, of course, the basic lore of linear algebra and calculus. For instance: the eigenvalues of a matrix of order n coincide with the zeros of a polynomial of order n, the secular determinant of the matrix; sets of polynomials, such as the classical (Hermite, Laguerre, and Jacobi) polynomials, may be identified as the eigenfunctions of linear differential operators; a matrix of order n is

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associated with a linear differential operator by projecting it in a finite-dimensional functional space, and if that space contains m eigenfunctions of the differential operator, the associated matrix possesses the corresponding m eigenvalues; and so on. We therefore hesitate to claim total novelty for the results reported below; indeed certain relationships with the standard problems of interpolation and mechanical quadrature (Ref. 9, Chaps. XIV and XV) are apparent. But we have not been able to locate in the literature any presentation of the basic results given below, nor of the specific findings they entail. Yet the applicative potential of these results appear vast. For instance, matrices having a known spectrum [such as (I.3) and those given below] should be useful for didactic purposes (even in secondary school) or for testing computer programs (note that the order n of these matrices may be arbitrarily large). Thus the fact that these results are not generally known supports our impression about their novelty and has provided one of the motivations for this presentation. [There are, of course, also other prescriptions to construct matrices with known eigenvalues; for instance one can "undiagonalize" a diagonal matrix by a canonical transformation, or one can use the connection with differential operators mentioned above. But these prescriptions are more cumbersome to carry out, especially if the order n is large, than the evaluation of explicit formulas such as (I.3).]

The paper is organized as follows. Section 1 contains the basic definitions and results. In Sec. 2 (which can be omitted in a first reading) these results are discussed in the framework of the standard theory relating matrices, differential operators, and orthogonal polynomials. In Sec. 3 matrices of order n, constructed in terms of n (or more) arbitrary numbers and having known eigenvalues and eigenvectors, are exhibited. In Sec. 4 matrices of order n having known eigenvalues and eigenvectors (and, in some cases, interesting algebraic properties) are exhibited, being constructed in terms of the nth roots of unity or of the n zeros of given polynomials. The result (I.6), and analogous representations for Laguerre, Legendre, Gegenbauer, and Jacobi polynomials, are also obtained. Section 5 concludes the paper by outlining some directions of future research that are suggested by these findings.

Clearly, the specific findings reported in Secs. 3 and 4 are merely instances of the kind of results that follows from the basic treatment of Sec. 1. Any diligent reader may easily find, in a similar manner, additional analogous results. But in the presentation of Secs. 3 and 4 we have also tried to cater to the casual reader, who is only interested in the application of these findings (for instance, to test a computer program). Thus we have striven (at the cost of some repetitiveness) to formulate the results self-consistently, so that they can also be utilized by a user who does not bother to read the whole paper and to master its notation; in particular, the reader who is only interested in using test matrices with known eigenvalues can proceed immediately to the relevant results given in Sec. 3.

1. BASIC DEFINITIONS AND RESULTS

Indices (and exponents) are indicated by lower case italic letters (j,k,l,m,p,q,r,s); the first few (j,k,l,m) range from 1 to n, the last few (q,r,s) from 0 to $n-1$; the index p is used for the generic nonnegative integer; n is a fixed integer, $n \geqslant 2$. Summations are generally over these respective ranges; but a prime appended to a summation symbol signifies omission of any singular term in the sum.

Lower (respectively upper) case *boldface* is used for vectors (respectively matrices), of order n; the generic vector $\mathbf{v}$ has components v_j, the generic matrix $\mathbf{M}$ has elements M_{jk}.

In Secs. 1, 2, and 3 the n *different* numbers x_j are arbitrary (possibly complex, except in Sec. 2). We use the notation $p_n(x)$ for the polynomial having the x_j's as zeros, and of course $p_n'(x)$ indicates its derivative:

$$p_n(x) = k_n \prod_{j=1}^{n} (x - x_j), \tag{1.1}$$

$$p_n'(x) = p_n(x) \sum_{j=1}^{n} (x - x_j)^{-1}. \tag{1.2}$$

The normalization constant k_n is unessential; it is introduced here for notational convenience in connection with the treatment of Sec. 2.

The vectors $\mathbf{u}$, $\mathbf{v}$, $\boldsymbol{\xi} \equiv \boldsymbol{\xi}^{(1)}$, and $\boldsymbol{\xi}^{(p)}$ are defined as follows:

$$u_j = 1, \tag{1.3}$$

$$v_j = [p'(x_j)]^{-1} = \Big[k_n \prod_{\substack{l=1\\ l\neq j}}^{n} (x_j - x_k)\Big]^{-1}, \tag{1.4}$$

$$\xi_j = \sum_{k=1}^{n}{}' (x_j - x_k)^{-1}, \quad \xi_j^{(p)} = \sum_{j=1}^{n}{}' (x_j - x_k)^{-p}. \tag{1.5}$$

The matrices $\mathbf{I}, \mathbf{J}, \mathbf{X}$, $\Xi \equiv \Xi^{(1)}$, $\Xi^{(p)}$, $\mathbf{Y}^{(1)} \equiv \mathbf{Y}, \mathbf{Y}^{(p)}$, and $\mathbf{Z}$ are defined as follows:

$$I_{jk} = \delta_{jk}, \quad J_{jk} = 1, \tag{1.6}$$

$$\mathbf{X} = \operatorname{diag}(x_j), \quad X_{jk} = \delta_{jk} x_j, \tag{1.7}$$

$$\Xi = \operatorname{diag}(\xi_j), \quad \Xi^{(p)} = \operatorname{diag}(\xi_j^{(p)}), \tag{1.8}$$

$$Y_{jk} = (1 - \delta_{jk})(x_j - x_k)^{-1}, \quad Y_{jk}^{(p)} = (1 - \delta_{jk})(x_j - x_k)^{-p}, \tag{1.9}$$

$$\mathbf{Z} = \Xi + \mathbf{Y},$$

$$Z_{jk} = \delta_{jk} \sum_{l=1}^{n}{}' (x_j - x_l)^{-1} + (1 - \delta_{jk})(x_j - x_k)^{-1}. \tag{1.10}$$

There are a number of trivial relationships satisfied by these matrices. We display the principal ones:

$$\mathbf{J}^2 = n\mathbf{J}, \quad \mathbf{J}\mathbf{u} = n\mathbf{u}, \tag{1.11}$$

$$\mathbf{J}\mathbf{Z} = 0, \tag{1.12}$$

$$\mathbf{J}\mathbf{X}\mathbf{Z} = (n-1)\,\mathbf{J}, \tag{1.13}$$

$$(\mathbf{Z}\mathbf{J})_{jk} = 2\xi_j, \tag{1.14a}$$

$$(\mathbf{X}\mathbf{Z}\mathbf{J})_{jk} = 2\xi_j x_j, \tag{1.14b}$$

$$[\mathbf{Z},\mathbf{X}] = \mathbf{I} - \mathbf{J}, \tag{1.15}$$

$$[\mathbf{X},\mathbf{Y}^{(p)}] = \mathbf{Y}^{(p-1)}, \tag{1.16}$$

$$\mathbf{Z}^2 = \Xi^2 - \Xi^{(2)} + 2\Xi\mathbf{Y} - 2\mathbf{Y}^{(2)}, \tag{1.17a}$$

$$(\mathbf{Z}^2)_{jk} = \delta_{jk}\Big\{\Big[\sum_{l=1}^{n}{}' (x_j - x_l)^{-1}\Big]^2 - \sum_{l=1}^{n}{}' (x_j - x_l)^{-2}\Big\} + 2(1 - \delta_{jk})(x_j - x_k)^{-1} \times \Big[\sum_{l=1}^{n}{}' (x_j - x_l)^{-1} - (x_j - x_k)^{-1}\Big]. \tag{1.17b}$$

$$(\mathbf{Z}^2)_{jk} = \delta_{jk} \sum_{l=1}^{n}{}' (x_j - x_l)^{-1} \sum_{m=1}^{n}{}' (x_j - x_m)^{-1}(1-\delta_{lm}) + 2(1-\delta_{jk})(x_j - x_k)^{-1} \times \sum_{l=1}^{n}{}' (x_j - x_l)^{-1}(1-\delta_{lk}) . \quad (1.17c)$$

The matrices $\mathbf{Z}$ and $\mathbf{Z}^2$ will play an important role; this motivates our display of three, clearly equivalent, versions of (1.17).

A fundamental role for all subsequent developments is played by the following Lemma.

Lemma 1.1: Let $P_q(x)$ be any polynomial of degree $q \leqslant n-1$; let the linear differential operator $\mathscr{F}$ be defined by

$$\mathscr{F} = \sum_{r=1}^{n-1} F_r(x) \frac{d^r}{dx^r}, \quad (1.18)$$

the functions $F_r(x)$ being entire but otherwise arbitrary; and let

$$Q(x) = \mathscr{F} \cdot P_q(x). \quad (1.19)$$

Define the matrix $\mathbf{F}$, of order n, by the formula

$$\mathbf{F} = \sum_{r=0}^{n-1} F_r(\mathbf{X})\, \mathbf{Z}^r, \quad (1.20)$$

obtained by replacing in (1.18) x by $\mathbf{X}$ and d/dx by $\mathbf{Z}$ [$\mathbf{X}$ and $\mathbf{Z}$ being defined by (1.7) and (1.10)]. There holds, then, the vector equation

$$Q(\mathbf{X})\,\mathbf{v} = \mathbf{F} P_q(\mathbf{X})\,\mathbf{v}, \quad (1.21)$$

with $\mathbf{v}$ defined by (1.4), (1.2), and (1.1).

To prove this Lemma it is convenient to go through the following results, some of which (see below) are in fact merely subcases of it.

Proposition 1.1:

$$\mathbf{J}\mathbf{X}^q\,\mathbf{v} = 0, \quad q = 0,1,\ldots,n-2. \quad (1.22)$$

Proof: Consider the function $f_q(z) = z^q/p_n(z)$ of the complex variable z [with $p_n(z)$ defined by (1.1)]. It is meromorphic in the whole complex z-plane, and it vanishes at least as $|z|^{-2}$ when $|z| \to \infty$. Therefore the sum of all its residues vanishes, since it coincides with the integral of $f_q(z)$ over a circle of diverging radius. But this yields precisely (1.22). Q.E.D.

Proposition 1.2:

$$\mathbf{J}\mathbf{X}^{n-1}\,\mathbf{v} = k_n^{-1}\,\mathbf{u}. \quad (1.23)$$

Proof: As above, with the obvious modification implied by the nonvanishing of the contour integral, whose evaluation yields the right-hand side (rhs) of (1.23). (This proposition is not needed for the proof of the Lemma, but it will be useful in the following.)

Proposition 1.3:

$$\mathbf{Z}\mathbf{X}^q\,\mathbf{v} = q\mathbf{X}^{q-1}\mathbf{v}, \quad q = 0,1,\ldots,n-1. \quad (1.24)$$

Proof: Same as above, but using the function $g_{jq}(z) = z^q/[(z-x_j)\,p_n(z)]$ in place of $f_q(z)$ [note that $g_{jq}(z)$ has $n-1$ simple poles at $z = x_k$, $k \neq j$, and one double pole at $z = x_j$].

Corollary 1.3.1: The matrix $\mathbf{Z}$ is nilpotent,

$$\mathbf{Z}^n = 0. \quad (1.25)$$

This result is not new.[3]

Proposition 1.4:

$$\mathbf{Z}^p\mathbf{X}^q\,\mathbf{v} = 0 \quad \text{if} \quad p > q, \quad q = 0,1,\ldots,n-1; \quad (1.26a)$$

$$\mathbf{Z}^p\mathbf{X}^q\,\mathbf{v} = [q!/(q-p)!]\,\mathbf{X}^{q-p}\,\mathbf{v} \quad \text{if} \quad 0 \leqslant p \leqslant q, \quad q = 0,1,\ldots,n-1. \quad (1.26b)$$

Proof: By elementary algebraic techniques or by recursion, using (1.24), (1.15), (1.12), and (1.22).

The validity of Lemma 1.1 is an elementary consequence of the last Proposition.

The main notion implied by Lemma 1.1 [or, for that matter, by (1.26)] is the existence of a correspondence between the matrix $\mathbf{Z}$ and the differential operator d/dx; $\mathbf{Z}$ acts on powers of $\mathbf{X}$ in the same way as d/dx acts on powers of x. This correspondence, however, does not hold as a matrix equation, but only after application to the basic vector $\mathbf{v}$; moreover, it holds only for powers of $\mathbf{X}$ that are less than n. But let us reemphasize that it holds for the matrices $\mathbf{X}$ and $\mathbf{Z}$ explicitly defined by (1.7) and (1.10) in terms of the n *arbitrary* numbers x_j.

2. MATRICES AS PROJECTIONS OF DIFFERENTIAL OPERATORS

In Sec. 1 a connection has been displayed that relates the matrix $\mathbf{Z}$, of degree n, defined by (1.10) in terms of the n arbitrary numbers x_j, to the differential operator d/dx acting in the functional space spanned by polynomials of degree $n-1$ or less. This suggests that $\mathbf{Z}$ be simply related to the projection of d/dx on an appropriate basis of that functional space. In this section we display this relation in the framework of the general theory relating matrices, differential operators, and orthogonal polynomials.

We assume in this section that the polynomial $p_n(x)$, defined in terms of the n arbitrary numbers x_j by (1.1), belongs to a set of polynomials $p_m(x)$, orthogonal with some appropriate weight $w(x)$:

$$\int_a^b dx\, w(x)\, p_{l-1}(x)\, p_{m-1}(x) = \delta_{lm}, \quad l,m = 1,2,\ldots,n+1. \quad (2.1)$$

Note that, for notational convenience, we have assumed these polynomials to be normalized. The quantities a and b in (2.1) need not be finite; but we assume for simplicity that they, as well as the weight $w(x)$, are real. Thus we restrict consideration in this section to the case when all the numbers x_j are real, and fall in the (possibly infinite) interval (a,b).

We now report, for the convenience of the reader, certain standard formulas for orthogonal polynomials,[9,10] that are used below:

$$\sum_{m=1}^{n} p_{m-1}(x)\, p_{m-1}(y) = (k_{n-1}/k_n)[\,p_n(x)\,p_{n-1}(y) - p_{n-1}(x)\,p_n(y)]/(x-y), \quad (2.2)$$

$$\sum_{m=1}^{n} [p_{m-1}(x)]^2 = (k_{n-1}/k_n)[p_n'(x)p_{n-1}(x) - p_{n-1}'(x)p_n(x)], \quad (2.3)$$

$$p_{m+1}(x) = (A_m x + B_m)\, p_m(x) - C_m\, p_{m-1}(x)\,, \quad (2.4)$$
$$A_m = k_{m+1}/k_m\,,$$
$$B_m = A_m(r_{m+1} - r_m), \quad C_m = A_m/A_{m-1}\,.$$

In these equations (and below) the quantities k_m and r_m are defined by

$$p_m(x) = k_m(x^m + r_m x^{m-1} + \cdots)\,. \quad (2.5)$$

We assume, for definiteness, k_m to be positive.

Alternative versions of some of the equations given below are obtained using the formula

$$p_{n-1}(x_j) = -[k_n^2/(k_{n-1}\, k_{n+1})]\, p_{n+1}(x_j)\,, \quad (2.6)$$

which is implied by (2.4) and (1.1).

We introduce now another set of orthonormal polynomials $p_{n-1}^{(j)}(x)$, all of them of degree $n-1$:

$$p_{n-1}^{(j)}(x) = c_j\, p_n(x)/(x - x_j), \quad j = 1,2,\ldots,n, \quad (2.7)$$

$$c_j = \{k_{n-1}\, p_{n-1}(x_j)/[k_n\, p_n'(x_j)]\}^{1/2}, \quad j = 1,2,\ldots,n, \quad (2.8)$$

$$\int_a^b dx\, w(x)\, p_{n-1}^{(j)}(x)\, p_{n-1}^{(k)}(x) = \delta_{jk}, \quad j,k = 1,2,\ldots,n. \quad (2.9)$$

It can be easily shown that the argument of the square root in (2.8) is always positive.

These polynomials possess the following properties:

$$p_{n-1}^{(j)}(x) = c_j\, k_n \prod_{\substack{l=1\\ l\neq j}}^{n} (x - x_l)\,, \quad (2.10)$$

$$p_{n-1}^{(j)}(x_k) = \delta_{jk}\, c_j k_n \prod_{\substack{l=1\\ l\neq j}}^{n} (x_j - x_l)\,, \quad (2.11a)$$

$$p_{n-1}^{(j)}(x_k) = \delta_{jk}\, c_j\, p_n'(x_j)\,, \quad (2.11b)$$

$$\sum_{j=1}^{n} \frac{p_{n-1}^{(j)}(x)}{c_j} = p_n'(x)\,, \quad (2.12)$$

$$\sum_{j=1}^{n} p_{n-1}^{(j)}(x)\, p_{n-1}^{(j)}(y) = \sum_{m=1}^{n} p_{m-1}(x)\, p_{m-1}(y)\,, \quad (2.13a)$$

$$\sum_{j=1}^{n} p_{n-1}^{(j)}(x)\, p_{n-1}^{(j)}(y) = \frac{k_{n-1}}{k_n}\, \frac{p_n(x)\, p_{n-1}(y) - p_{n-1}(x) p_n(y)}{(x-y)}\,, \quad (2.13b)$$

$$\sum_{j=1}^{n} [p_{n-1}^{(j)}(x)]^2 = \frac{k_{n-1}}{k_n}\, [p_n'(x)\, p_{n-1}(x) - p_{n-1}'(x)\, p_n(x)]\,, \quad (2.14)$$

$$\sum_{m=1}^{n} p_{m-1}(x_j)\, p_{m-1}(x) = c_j\, p_n'(x_j)\, p_{n-1}^{(j)}(x)\,, \quad (2.15)$$

$$\sum_{l=1}^{n} p_{n-1}^{(l)}(x_j)\, p_{n-1}^{(l)}(x_k) = \delta_{jk}\, [p_{n-1}^{(j)}(x_j)]^2\,. \quad (2.16)$$

It is also of interest to report the linear transformations relating the orthonormal polynomials $p_{m-1}(x)$, $m = 1,2,\ldots,n$ (of degrees $0,1,\ldots,n-1$) to the polynomials $p_{n-1}^{(j)}(x), j = 1,2,\ldots,n$ (all of them of degree $n-1$):

$$p_{n-1}^{(j)}(x) = \sum_{m=1}^{n} u_m^{(j)}\, p_{m-1}(x), \quad j = 1,2,\ldots,n, \quad (2.17)$$

$$p_{m-1}(x) = \sum_{j=1}^{n} u_m^{(j)}\, p_{n-1}^{(j)}(x), \quad m = 1,2,\ldots,n. \quad (2.18)$$

The quantities $u_m^{(j)}$ satisfy the orthogonality and completeness relations

$$\sum_{m=1}^{n} u_m^{(j)} u_m^{(k)} = \delta_{jk}\,, \quad j,k = 1,2,\ldots,n, \quad (2.19)$$

$$\sum_{j=1}^{n} u_l^{(j)} u_m^{(j)} = \delta_{lm}, \quad l,m = 1,2,\ldots,n, \quad (2.20)$$

and are explicitly given by the formula

$$u_m^{(j)} = p_{m-1}(x_j)/[c_j\, p_n'(x_j)]\,. \quad (2.21)$$

These equations, (2.7)–(2.21), are not new (see Chaps. XIV and XV of Ref. 9); indeed the quantities c_j, see (2.8), are related to the Christoffel numbers λ_j [see Eq. (3.4.7) of Ref. 9] by

$$c_j = (k_{n-1}/k_n)\, p_{n-1}(x_j)\, \lambda_j^{1/2} = [p_n'(x_j)]^{-1}\, \lambda_j^{-1/2}\,. \quad (2.22)$$

However, for completeness, we provide a terse proof of them in Appendix A.

The formulas (2.19) and (2.20) suggest the introduction of an n-dimensional vector space, spanned by the orthogonal set of unit vectors $\tilde{\mathbf{u}}^{(m)}$, $m = 1,2,\ldots,n$, of components $\tilde{\mathbf{u}}_j^{(m)}$,

$$\tilde{\mathbf{u}}_j^{(m)} = u_m^{(j)}, \quad j,m = 1,2,\ldots,n. \quad (2.23)$$

Then clearly [with obvious notation, see (2.19) and (2.20)]

$$(\tilde{\mathbf{u}}^{(l)}, \tilde{\mathbf{u}}^{(m)}) = \delta_{lm}\,, \quad (2.24)$$

$$\sum_{l=1}^{n} \tilde{\mathbf{u}}^{(l)} \otimes \tilde{\mathbf{u}}^{(l)} = \mathbf{I}\,. \quad (2.25)$$

The motivation for using the definition (2.23) is that this allows a neat translation of equations valid in the functional space of the original orthogonal polynomials $p_m(x)$ into formulas in the n-dimensional vector space we have just introduced. For instance, to the eigenvalue equation

$$\mathscr{A}\, p_{p-1}(x) = a_p\, p_{p-1}(x), \quad p = 1,2,\cdots, \quad (2.26)$$

$\mathscr{A}$ being, say, a differential operator, there corresponds the vector equation

$$\mathbf{A}\, \tilde{\mathbf{u}}^{(m)} = a_m\, \tilde{\mathbf{u}}^{(m)}, \quad m = 1,2,\ldots,n\,, \quad (2.27)$$

with the matrix $\mathbf{A}$ defined by

$$A_{jk} = \int_a^b dx\, w(x)\, p_{n-1}^{(j)}(x)\, \mathscr{A}\, p_{n-1}^{(k)}(x)\,; \quad (2.28)$$

to the raising and lowering operator formulas

$$\mathscr{A}^{(\pm)} p_{p-1}(x) = \alpha_p^{(\pm)}\, p_{-1\pm 1}(x), \quad \alpha_1^{(-)} = 0, \quad p = 1,2,\cdots, \quad (2.29)$$

there correspond the vector equations

$$\mathbf{A}^{(-)} \tilde{\mathbf{u}}^{(m)} = \alpha_m^{(-)}\, \tilde{\mathbf{u}}^{(m-1)}, \quad m = 1,2,\ldots,n, \quad (2.30a)$$

$$\mathbf{A}^{(+)}\, \tilde{\mathbf{u}}^{(m)} = (\alpha_m^{(+)} - \delta_{nm}\alpha_n^{(+)})\, \tilde{\mathbf{u}}^{(m+1)}, \quad m = 1,2,\ldots n, \quad (2.30b)$$

again with the matrices $\mathbf{A}^{(\pm)}$ defined by

$$A_{jk}^{(\pm)} = \int_a^b dx\, w(x)\, p_{n-1}^{(j)}(x)\, \mathscr{A}^{(\pm)} p_{n-1}^{(k)}(x)\,; \quad (2.31)$$

and so on. Note the extra term in the rhs of (2.30b) as compared to (2.29), implying

$$\mathbf{A}^{(+)}\, \tilde{\mathbf{u}}^{(n)} = 0\,; \quad (2.32)$$

its appearance is, of course, related to the fact that the space spanned by the vectors $\tilde{\mathbf{u}}^{(m)}$, $m = 1,2,...,n$ [or, equivalently, by the orthogonal polynomials $p_{n-1}^{(j)}(x), j = 1,2,...,n$] is n-dimensional, while the space spanned by the orthogonal polynomials $p_{p-1}(x)$, $p = 1,2, \cdots$, is infinite-dimensional.

Clearly the matrices $\mathbf{A}$ and $\mathbf{A}^{(\pm)}$ can also be expressed by the formulas

$$\mathbf{A} = \sum_{m=1}^{n} a_m \, \tilde{\mathbf{u}}^{(m)} \otimes \tilde{\mathbf{u}}^{(m)}, \tag{2.33}$$

$$\mathbf{A}^{(-)} = \sum_{m=2}^{n} \alpha_m^{(-)} \, \tilde{\mathbf{u}}^{(m-1)} \otimes \tilde{\mathbf{u}}^{(m)}, \tag{2.34a}$$

$$\mathbf{A}^{(+)} = \sum_{m=1}^{n-1} \alpha_m^{(+)} \, \tilde{\mathbf{u}}^{(m+1)} \otimes \tilde{\mathbf{u}}^{(m)}. \tag{2.34b}$$

These formulas contain no integration [in contrast to (2.28) and (2.31)]; but they involve all the polynomials $p_{m-1}(x)$, $m = 1,2,...,n$, [evaluated at the points x_j; see (2.21) and (2.23)].

It is now natural to introduce the matrices $\tilde{\mathbf{X}}$ and $\tilde{\mathbf{Z}}$ via the definitions

$$\tilde{X}_{jk} = \int_a^b dx \, w(x) \, p_{n-1}^{(j)}(x) \, x \, p_{n-1}^{(k)}(x), \tag{2.35}$$

$$\tilde{Z}_{jk} = \int_a^b dx \, w(x) \, p_{n-1}^{(j)}(x) \left(\frac{d}{dx}\right) p_{n-1}^{(k)}(x). \tag{2.36}$$

The (very simple) relation of these matrices to the matrices $\mathbf{X}$ and $\mathbf{Z}$ introduced in the preceding section is specified by the following

Proposition 2.1: Let the matrices $\mathbf{X}$ and $\mathbf{Z}$, of order n, be defined, in terms of the n arbitrary numbers x_j, by (1.7) and (1.10); and let the matrices $\tilde{\mathbf{X}}$ and $\tilde{\mathbf{Z}}$ be defined, in terms of the same numbers x_j, by (2.35) and (2.36) [with (2.7), (2.8), (2.5), and (1.1)]. There holds then the relations

$$\tilde{\mathbf{X}} = \mathbf{X} = \mathbf{C}^{-1}\mathbf{X}\mathbf{C}, \tag{2.37}$$

$$\tilde{\mathbf{Z}} = \mathbf{C}^{-1}\mathbf{Z}\mathbf{C}, \tag{2.38}$$

with the diagonal matrix $\mathbf{C}$ defined by

$$\mathbf{C} = \mathrm{diag}(c_j), \quad C_{jk} = \delta_{jk} c_j, \tag{2.39}$$

where the c_j's are defined by (2.8).

Proof: The first part, namely (2.37), is a well-known result[9] whose proof need not be reported (it is analogous to, but more straightforward than, the proof of the second part); note that the second equality in (2.37) is trivially equivalent to the first, since $\mathbf{X}$ and $\mathbf{C}$ obviously commute (they are both diagonal). To prove (2.38) we note that (2.36) can be rewritten in the form

$$\tilde{Z}_{jk} = \int_a^b dx \, w(x) \, p_{n-1}^{(j)}(x) \, p_{n-1}^{(k)}(x) \sum_{\substack{l=1 \\ l \neq k}}^{n} (x - x_l)^{-1}, \tag{2.40}$$

where we have used the formula

$$\frac{dp_{n-1}^{(k)}(x)}{dx} = p_{n-1}^{(k)}(x) \sum_{\substack{l=1 \\ l \neq k}}^{n} (x - x_l)^{-1}, \tag{2.41}$$

implied by (2.10). Now use of the identity

$$\sum_{\substack{l=1 \\ l \neq k}}^{n} (x - x_l)^{-1} \equiv \sum_{l=1}^{n}{}' (x_k - x_l)^{-1} - (x - x_k) \sum_{l=1}^{n}{}' (x_k - x_l)^{-1} (x - x_l)^{-1}, \tag{2.42}$$

yields

$$\tilde{Z}_{jk} = \delta_{jk} \sum_{l=1}^{n}{}' (x_j - x_l)^{-1} - \sum_{l=1}^{n}{}' (x_k - x_l)^{-1} \left(\frac{c_k}{c_l}\right) \times \int_a^b dx \, w(x) \, p_{n-1}^{(j)}(x) \, p_{n-1}^{(l)}(x). \tag{2.43}$$

To obtain the first term in the rhs, (2.9) has been used, while to get the second term, (2.7) has been used twice. Now using once more (2.9) there obtains (2.38). Q.E.D.

If the weight $w(x)$ has the property to vanish at both ends of the interval (a,b), as is, for instance, the case if the polynomial $p_m(x)$ coincides with the Hermite polynomial $H_n(x)$, or with the generalized Laguerre polynomial $L_n^{\alpha}(x)$ with $\alpha > 0$, or with the Jacobi polynomial $p_n^{(\alpha,\beta)}(x)$ with $\alpha > 0$ and $\beta > 0$ (here, and throughout this paper, we use for orthogonal polynomials the notation of Ref. 10), then by performing a partial integration in the rhs of (2.36) and using (2.7), (2.38), and (1.10) we obtain the formulas

$$(x_j - x_k)^{-1}(c_j^{-2} - c_k^{-2}) = -\tfrac{1}{2} \int_a^b dx \, w'(x) \, p_n^2(x) / [(x - x_j)(x - x_k)], \quad j,k = 1,2,...,n, \; j \neq k, \tag{2.44}$$

$$\xi_j = \sum_{k=1}^{n}{}' (x_j - x_k)^{-1} = -\tfrac{1}{2} \int_a^b dx w'(x) \, [p_n(x)/(x - x_j)]^2. \tag{2.45}$$

These formulas provide a connection between the zeros of the polynomial $p_n(x)$ and the derivative of the weight $w(x)$. Note that (2.45) contains no additional constant besides the x_j's [recall that the polynomials $p_m(x)$ are, by assumption, normalized, see (2.1)], while (2.44) can be compared with the formula

$$c_j^{-2} = \int_a^b dx \, w(x) [p_n(x)/(x - x_j)]^2, \tag{2.46}$$

which is implied by (2.22) together with Eq. (3.4.6) of Ref. 9. Also note that this last formula, together with (2.44), yields the remarkable equation

$$\int_a^b dx \, \{w(x)[(x - x_j)^{-1} + (x - x_k)^{-1}] + \tfrac{1}{2} w'(x)\} \times \left(\frac{p_n^2(x)}{(x - x_j)(x - x_k)}\right) = 0, \quad j,k = 1,2,...,n, \quad j \neq k, \tag{2.47}$$

valid for the orthogonal polynomial $p_n(x)$.

The main result of this section is displayed by Proposition 2.1. This finding, together with the rest of the discussion in this section, shows how the main result of Sec. 1 can be set in the framework of the standard theory relating matrices and linear differential operators. The content of Lemma 1.1 should nevertheless be considered nontrivial, in view of the simple and explicit form of the matrix $\mathbf{Z}$, see (1.10). This is confirmed by the implications that follow quite directly from

Lemma 1.1, as exemplified by the results reported in the following two sections.

3. PROPERTIES OF CERTAIN MATRICES CONSTRUCTED WITH ARBITRARY NUMBERS

The following result is an immediate consequence of Lemma 1.1.

Lemma 3.1: Let the linear differential operator

$$\mathscr{F} = \sum_{r=0}^{n-1} F_r(x) \frac{d^r}{dx^r}, \tag{3.1}$$

possess $m \leqslant n$ distinct eigenvalues f_l, $l = 1,2,...,m$, the corresponding eigenfunctions $P^{(l)}(x)$ being polynomials of degree $n-1$ or less:

$$\mathscr{F} P^{(l)}(x) = f_l P^{(l)}(x), \quad l = 1,2,...,m \leqslant n,$$

$$P^{(l)}(x) = \sum_{q=0}^{n-1} a_q^{(l)} x^q. \tag{3.2}$$

Then the matrix of order n

$$\mathbf{F} = \sum_{r=0}^{n-1} F_r(\mathbf{X}) \mathbf{Z}^r, \tag{3.3}$$

with $\mathbf{X}$ and $\mathbf{Z}$ defined by (1.7) and (1.10) in terms of the n arbitrary numbers x_j, has the same eigenvalues f_l and the (unnormalized) eigenvectors

$$\mathbf{v}^{(l)} = P^{(l)}(\mathbf{X})\, \mathbf{v}, \quad l = 1,2,...,m \leqslant n, \tag{3.4}$$

with $\mathbf{v}$ defined by (1.4) [with (1.2) and (1.1)]:

$$\mathbf{F}\mathbf{v}^{(l)} = f_l \mathbf{v}^{(l)}, \quad l = 1,2,...,m \leqslant n. \tag{3.5}$$

The extension of this result to the case with multiple eigenvalues requires the appropriate qualifications about the linear independence of eigenfunctions and eigenvectors, but is otherwise straightforward.

Note that we are assuming neither the differential operator nor the corresponding matrix to be Hermitian. Indeed the results of Sec. 1, and most of those of this and the following sections, do not require the introduction of a scalar product, either in the functional space nor in the vector space.

Many matrices with (fully or partly) known spectrum can now be easily constructed using Lemma 3.1 and standard results for differential operators with polynomial eigenfunctions. We report below a few examples; in some cases we also display the additional algebraic results that follow from the possibility, implied by Lemma 1.1, to translate the properties of a differential operator (for instance, to act as a raising or lowering operator on the eigenfunctions of the differential operator $\mathscr{F}$) into analogous properties of the corresponding matrix.

Proposition 3.1: The matrix of order n

$$\mathbf{N} = \mathbf{X}\mathbf{Z}, \tag{3.6}$$

with $\mathbf{X}$ and $\mathbf{Z}$ defined by (1.7) and (1.10) in terms of the n arbitrary numbers x_j, has the first n nonegative integers as eigenvalues, and the corresponding (unnormalized) eigenvectors are

$$\mathbf{v}^{(m)} = \mathbf{X}^{m-1}\mathbf{v}, \quad m = 1,2,...,n, \tag{3.7}$$

with $\mathbf{v}$ defined by (1.4) [with (1.2) and (1.1)]:

$$\mathbf{N}\mathbf{v}^{(m)} = (m-1)\, \mathbf{v}^{(m)}, \quad m = 1,2,...,n. \tag{3.8}$$

There hold, moreover, the following equations:

$$\mathbf{Z}\mathbf{v}^{(m)} = (m-1)\, \mathbf{v}^{(m-1)}, \quad m = 1,2,...,n, \tag{3.9}$$

$$\mathbf{X}\mathbf{v}^{(m)} = \mathbf{v}^{(m+1)}, \quad m = 1,2,...,n-1, \tag{3.10}$$

$$\mathbf{J}\mathbf{v}^{(m)} = \delta_{mn}\, k_n^{-1}\mathbf{u}, \quad m = 1,2,...,n, \tag{3.11}$$

$$[\mathbf{Z},\mathbf{N}] = \mathbf{Z}, \tag{3.12}$$

$$[\mathbf{N},\mathbf{X}] = \mathbf{X}(\mathbf{I} - \mathbf{J}), \tag{3.13}$$

with $\mathbf{I}$, $\mathbf{J}$, k_n and $\mathbf{u}$ defined by (1.6), (1.1), and (1.3).

These results are not new[3] [indeed the definition (3.6) of $\mathbf{N}$ coincides with (I.3)]; in the present context they correspond to the differential operator $\mathscr{F} = x\, d/dx$, with eigenfunctions x^p.

Proposition 3.2: The matrix of order n

$$\mathbf{N}^{(H)} = \mathbf{X}\mathbf{Z} - \tfrac{1}{2}\mathbf{Z}^2, \tag{3.14}$$

with $\mathbf{X}$ and $\mathbf{Z}$ defined in terms of the n arbitrary numbers x_j by (1.7) and (1.10) [and $\mathbf{Z}^2$ defined explicitly by (1.17)] has the first n nonnegative integers as eigenvalues, and the corresponding (unnormalized) eigenvectors are

$$\mathbf{v}^{(H)(m)} = H_{m-1}(\mathbf{X})\, \mathbf{v}, \quad m = 1,2,...,n, \tag{3.15}$$

with $H_p(x)$ the Hermite polynomial[9,10] of degree p and $\mathbf{v}$ defined by (1.4) [with (1.2) and (1.1)]:

$$\mathbf{N}^{(H)}\mathbf{v}^{(H)(m)} = (m-1)\, \mathbf{v}^{(H)(m)}, \quad m = 1,2,...,n. \tag{3.16}$$

There hold, moreover, the following equations:

$$\mathbf{Z}\mathbf{v}^{(H)(m)} = 2(m-1)\, \mathbf{v}^{(h)(m-1)}, \quad m = 1,2,..,n, \tag{3.17}$$

$$(2\mathbf{X} - \mathbf{Z})\, \mathbf{v}^{(H)(m)} = \mathbf{v}^{(H)(m+1)}, \quad m = 1,2,...,n-1, \tag{3.18a}$$

$$(2\mathbf{X} - \mathbf{Z})\mathbf{v}^{(H)(n)} = H_n(\mathbf{X})\mathbf{v}, \tag{3.18b}$$

$$\mathbf{J}\mathbf{v}^{(H)(m)} = \delta_{mn}(2^{n-1}/k_n)\mathbf{u}. \tag{3.19}$$

Note that the vector appearing in the rhs of (3.18b) is generally a linear combination of the n vectors $\mathbf{v}^{(H)(m)}$, with coefficients depending on the numbers x_j. If the x_j's coincide with the n zeros of the Hermite polynomial of order n, then the rhs of (3.18b) vanishes (this case is considered in Sec. 4).

Clearly the results of this Proposition are an immediate consequence of the Lemmas and of the well-known formulas[9,10]

$$xH_p'(x) - \tfrac{1}{2}H_p''(x) = pH_p(x), \quad H_p'(x) = 2pH_{p-1}(x),$$

$$2xH_p(x) - H_p'(x) = H_{p+1}(x).$$

Proposition 3.3: The matrix of order n

$$\mathbf{N}^{(L)} = [\mathbf{X} - (1+\alpha)\mathbf{I}]\mathbf{Z} - \mathbf{X}\mathbf{Z}^2, \tag{3.20}$$

with $\mathbf{I}$ the unit matrix, α any arbitrary number, and $\mathbf{X}$ and $\mathbf{Z}$ defined, in terms of the n arbitrary numbers x_j, by (1.7) and (1.10) [and $\mathbf{Z}^2$ defined explicitly by (1.17)] has the first n nonnegative integers as eigenvalues, and the corresponding (unnormalized) eigenvectors are

$$\mathbf{v}^{(L)(m)} = L_{m-1}^{\alpha}(\mathbf{X})\, \mathbf{v}, \quad m = 1,2,...,n, \tag{3.21}$$

with $L_p^{\alpha}(x)$ the Laguerre polynomial[10] of degree p and $\mathbf{v}$ defined by (1.4) [with (1.2) and (1.1)]:

$$\mathbf{N}^{(L)}\mathbf{v}^{(L)(m)} = (m-1)\mathbf{v}^{(L)(m)}, m = 1,2,...,n. \tag{3.22}$$

There hold, moreover, the following equations:

$$\mathbf{L}^{(-)}\mathbf{v}^{(L)(m)} = (m-1+\alpha)\, \mathbf{v}^{(L)(m-1)}, m = 2,3,...,n, \tag{3.23a}$$

$$\mathbf{L}^{(-)}\mathbf{v}^{(L)(1)} \equiv \mathbf{L}^{(-)}\mathbf{v} = 0\,, \tag{3.23b}$$

$$\mathbf{L}^{(+)}\mathbf{v}^{(L)(m)} = m\mathbf{v}^{(L)(m+1)}, \quad m = 1,2,...,n-1\,, \tag{3.24a}$$

$$\mathbf{L}^{(+)}\mathbf{v}^{(L)(n)} = nL_n^{\alpha}(\mathbf{X})\mathbf{v}, \tag{3.24b}$$

with

$$\mathbf{L}^{(-)} = -\,[\mathbf{XZ} + (1+\alpha)\,\mathbf{I}]\,\mathbf{Z}\,, \tag{3.25a}$$

$$\mathbf{L}^{(+)} = (1+\alpha)\mathbf{I} - \mathbf{X} - [(1+\alpha)\mathbf{I} - 2\mathbf{X}]\mathbf{Z} - \mathbf{XZ}^2; \tag{3.25b}$$

and

$$\mathbf{J}\mathbf{v}^{(L)(m)} = \delta_{nm}(-)^{n-1}[(n-1)!\,k_n]^{-1}\,\mathbf{u}\,. \tag{3.26}$$

Analogous remarks to those given after (3.19) apply to (3.24b). Note that the spectrum of the matrix $\mathbf{N}^{(L)}$ (3.20) is independent, not only of the n numbers x_j, but of α as well.

Corollary 3.3.1: The matrix $\mathbf{L}^{(-)}$, of order n, defined in terms of the $n+1$ arbitrary numbers x_j and α by (3.25), (1.6), (1.7), (1.10), and (1.17), is nilpotent:

$$[\mathbf{L}^{(-)}]^n = 0. \tag{3.27}$$

The formula corresponding, via Lemma 3.1, to (3.22), is the differential equation satisfied by the (generalized) Laguerre polynomials[10]

$$(x+\alpha-1)\,y_m' - xy_m'' = (m-1)\,y_m, \quad y_m \equiv L_{m-1}^{\alpha}(x)\,, \tag{3.28}$$

while those corresponding to (3.23) and (3.24) are consequences of the formulas[10]

$$\begin{aligned} xy_m' &= (m-1)\,y_m - (m-1+\alpha)\,y_{m-1} \\ &= my_{m+1} + (x-m-\alpha)\,y_m\,, \end{aligned}$$

$$y_m \equiv L_{m-1}^{\alpha}(x)\,, \tag{3.29}$$

together with (3.28) or (3.22).

Proposition 3.4: The matrix of order n

$$\mathbf{N}^{(J)} = [(\alpha-\beta)\,\mathbf{I} + (\alpha+\beta+2)\;\mathbf{X}]\;\mathbf{Z} + (\mathbf{X}^2 - \mathbf{I})\,\mathbf{Z}^2\,, \tag{3.30}$$

with $\mathbf{I}$ the unit matrix, α and β any arbitrary numbers, and $\mathbf{X}$ and $\mathbf{Z}$ defined, in terms of the n arbitrary numbers x_j, by (1.7) and (1.10) [and $\mathbf{Z}^2$ defined explicitly by (1.17)], has the n eigenvalues $(m-1)(m+\alpha+\beta)$, $m = 1,2,...,n$, and the corresponding (unnormalized) eigenvectors are

$$\mathbf{v}^{(J)(m)} = P_{m-1}^{(\alpha,\beta)}(\mathbf{X})\,\mathbf{v}, \quad m = 1,2,...,n\,, \tag{3.31}$$

with $P_p^{(\alpha,\beta)}(x)$ the Jacobi polynomial[9,10] of degree p and $\mathbf{v}$ defined by (1.4) [with (1.2) and (1.1)]:

$$\mathbf{N}^{(J)}\,\mathbf{v}^{(J)(m)} = (m-1)(m+\alpha+\beta)\,\mathbf{v}^{(J)(m)}, \quad m = 1,2,...,n\,. \tag{3.32}$$

There hold, moreover, the following equations:

$$\begin{aligned} &(2m+\alpha+\beta)(2m+\alpha+\beta-1)(2m+\alpha+\beta-2)\;\mathbf{X}\mathbf{v}^{(J)(m)} \\ &\quad = 2m(2m+\alpha+\beta)(2m+\alpha+\beta-2)\;\mathbf{v}^{(J)(m+1)} \\ &\qquad + (\beta^2-\alpha^2)(2m+\alpha+\beta-1)\;\mathbf{v}^{(J)(m)} \\ &\qquad + 2(m+\alpha-1)(m+\beta-1)(2m+\alpha+\beta) \\ &\qquad \times \mathbf{v}^{(J)(m-1)}, \quad m = 2,3,...,n-1\,, \end{aligned} \tag{3.33a}$$

$$\begin{aligned} &(2m+\alpha+\beta)(2m+\alpha+\beta-1)(2m+\alpha+\beta-2)\;\mathbf{Z}\mathbf{v}^{(J)(m)} \\ &\quad = -2m(m-1)(2m+\alpha+\beta)(2m+\alpha+\beta-2) \\ &\qquad \times \mathbf{v}^{(J)(m+1)} + 2(\alpha-\beta)(m-1)(m+\alpha+\beta) \\ &\qquad \times (2m+\alpha+\beta-1)\;\mathbf{v}^{(J)(m)} + 2(m+\alpha-1) \\ &\qquad \times (m+\beta-1)(m+\alpha+\beta)(2m+\alpha+\beta)\;\mathbf{v}^{(J)(m-1)}, \\ &\qquad m = 2,3,...,n-1\,, \end{aligned} \tag{3.33b}$$

$$\mathbf{J}\mathbf{v}^{(J)(m)} = \delta_{nm}\;2^{-(n+1)}\binom{2(n-1)+\alpha+\beta}{n-1}\,k_n^{-1}\,\mathbf{u}\,. \tag{3.34}$$

Note that the spectrum of the matrix $\mathbf{N}^{(J)}$ depends only on $\alpha+\beta$ (it is independent not only of the n numbers x_j, but of the difference $\alpha-\beta$ as well).

The differential equations corresponding to (3.32) – (3.34) are standard equations for the Jacobi polynomials $P_p^{(\alpha,\beta)}(x)$,[9,10] which are not reported here.

We provide now some more examples of matrices, always given by simple explicit formulas in terms of n (or more) arbitrary numbers, whose spectrum is only partially known.

Proposition 3.5: The matrix of order n

$$\tilde{\mathbf{N}}^{(H)} = -q\mathbf{I} - \tfrac{1}{2}q(q+1)\,\mathbf{X}^{-2} + (\mathbf{X} + q\mathbf{X}^{-1})\,\mathbf{Z} - \tfrac{1}{2}\mathbf{Z}^2\,, \tag{3.35}$$

with q any nonnegative integer less than n,

$$q = 0,1,2,...,n-1\,, \tag{3.36}$$

$\mathbf{I}$ the unit matrix, $\mathbf{X}$ defined by (1.7) in terms of the n numbers x_j (arbitrary except for the restrictions $x_j \neq x_k$, $x_j \neq 0$), $\mathbf{Z}$ (and $\mathbf{Z}^2$) defined by (1.10) [and (1.17)], has the first $n-q$ nonnegative integers as eigenvalues, and the corresponding (unnormalized) eigenvectors are

$$\tilde{\mathbf{v}}^{(H)(m)} = \mathbf{X}^q\,H_{m-1}(\mathbf{X})\,\mathbf{v}, \quad m = 1,2,...,n-q\,, \tag{3.37}$$

with $H_p(x)$ the Hermite polynomial[9,10] of degree p and $\mathbf{v}$ defined by (1.14) [with (1.2) and (1.1)]:

$$\tilde{\mathbf{N}}^{(H)}\,\tilde{\mathbf{v}}^{(H)(m)} = (m-1)\,\tilde{\mathbf{v}}^{(H)(m)}, \quad m = 1,2,...,n-q\,. \tag{3.38}$$

We have, moreover, the equation

$$\mathbf{J}\mathbf{v}^{(H)(m)} = \delta_{m,n-q}(2^{m-1}/k_n)\,\mathbf{u}\,. \tag{3.39}$$

Note that only if $q = 0$ is the complete spectrum of $\tilde{N}^{(H)}$ given [indeed in this case $\tilde{N}^{(H)} = N^{(H)}$; see (3.14)]; for instance, for $n = 2$ and $q = 1$ the matrix $\tilde{N}^{(H)}$ has, in addition to the eigenvalue 0 [corresponding to $m = 1$; see (3.38)], the eigenvalue $1 - x_1^{-2} - x_2^{-2} - (x_1x_2)^{-1}$.

The differential formula corresponding to (3.38) reads, of course,

$$y'' - 2(x + q/x)\,y' + [2(m+q-1) + q(q+1)\,x^{-2}]\,y = 0,$$
$$y \equiv x^q H_{m-1}(x)\,. \tag{3.40a}$$

Another example is obtained from the differential equation

$$xy'' + (1-\alpha-x)\,y' + [q + r - q(\alpha+q)/x]\,y = 0,$$
$$y \equiv x^q\,L_r^{\alpha+2q}(x)\,. \tag{3.40b}$$

Here and below $L_p^{\alpha}(x)$ is the (generalized) Laguerre polynomial.[10] It can be formulated as follows.

Proposition 3.6. The matrix $\mathbf{N}^{(L)}$ defined by (3.20), satisfies the vector equation

$$[\mathbf{N}^{(L)} + q(q+\alpha)\,\mathbf{X}^{-1} - (q+r)\mathbf{I}]\;\mathbf{X}^q\,L_r^{\alpha+2q}(\mathbf{X})\,\mathbf{v} = 0\,, \tag{3.41}$$

provided none of the (otherwise arbitrary) n different numbers x_j vanishes and q and r are two nonnegative integers whose sum is less than n,

$$x_j \neq 0, \quad j=1,2,...,n; \quad q=0,1,...,n-1; \quad r=0,1,...,n-1; \quad q+r<n. \tag{3.42}$$

Immediate consequences of this Proposition are the following two Corollaries (in addition to Proposition 3.3).

Corollary 3.6.1: the matrix of order n

$$\tilde{\mathbf{N}}^{(L)} = -q\mathbf{I} + q(q+\alpha)\mathbf{X}^{-1} + [\mathbf{X} - (1+\alpha)\mathbf{I}]\mathbf{Z} - \mathbf{X}\mathbf{Z}^2, \tag{3.43}$$

{with α arbitrary, q any nonnegative integer less than n,

$$q=0,1,...,n-1, \tag{3.44}$$

$\mathbf{I}$ the unit matrix, $\mathbf{X}$ defined by (1.7) in terms of the n numbers x_j (arbitrary except for the restrictions $x_j \neq x_k, x_j \neq 0$), $\mathbf{Z}$ (and $\mathbf{Z}^2$) defined by (1.10) [and (1.17)]}, has the first $n-q$ nonnegative integers as eigenvalues and the corresponding (unnormalized) eigenvectors are

$$\tilde{\mathbf{v}}^{(L)(m)} = \mathbf{X}^q L_{m-1}^{\alpha+2q}(\mathbf{X})\,\mathbf{v}, \quad m=1,2,...,n-q, \tag{3.45}$$

with $L_p^{\alpha}(x)$ the (generalized) Laguerre polynomial[10] of degree p and $\mathbf{v}$ defined by (1.4) [with (1.2) and (1.1)]:

$$\tilde{\mathbf{N}}^{(L)}\tilde{\mathbf{v}}^{(L)(m)} = (m-1)\,\tilde{\mathbf{v}}^{(L)(m)}, \quad m=1,2,...,n-q. \tag{3.46}$$

There holds, moreover, the equation

$$\mathbf{J}\tilde{\mathbf{v}}^{(L)(m)} = \delta_{m,n-q}(-)^{m-1}[(m-1)!\,k_n]^{-1}\,\mathbf{u}. \tag{3.47}$$

Note that only if $q=0$ is the complete spectrum of $\tilde{N}^{(L)}$ determined {in this case $\tilde{N}^{(L)}$ reduces to $N^{(L)}$; see (3.20); indeed $\tilde{N}^{(L)} = -q[\mathbf{I} - (q+\alpha)\mathbf{X}^{-1}] + \mathbf{N}^{(L)}$}. For instance, for $n=2$ and $q=1$ the matrix $\tilde{\mathbf{N}}^{(L)}$ has, in addition to the eigenvalue 0 [corresponding to $m=1$; see (3.46)], the eigenvalue $-1+(\alpha+1)(x_1^{-1}+x_2^{-1})$.

Corollary 3.6.2: The matrix of order n

$$\hat{\mathbf{N}}^{(L)} = (n-1-q)\,\mathbf{X} + \mathbf{X}[(1+\alpha)\mathbf{I} - \mathbf{X}] + \mathbf{X}^2\mathbf{Z}^2, \tag{3.48}$$

{with α arbitrary, q any nonnegative integer less than n,

$$q=0,1,...,n-1, \tag{3.49}$$

$\mathbf{I}$ the unit matrix, $\mathbf{X}$, $\mathbf{Z}$ (and $\mathbf{Z}^2$) defined in terms of the n numbers x_j by (1.7), (1.10) [and (1.17)]}, has the $n-q$ eigenvalues $(m-1)(m-1+\alpha)$, $m=1,2,...,n-q$, and the corresponding (unnormalized) eigenvectors are

$$\hat{\mathbf{v}}^{(L)(m)} = \mathbf{X}^{m-1} L_{n-q-m}^{\alpha+2(m-1)}(\mathbf{X})\,\mathbf{v}, \quad m=1,2,...,n-q, \tag{3.50}$$

with $L_p^{\alpha}(x)$ the (generalized) Laguerre polynomial[10] of degree p and $\mathbf{v}$ defined by (1.4) [with (1.2) and (1.1)]:

$$\hat{N}^{(L)}\hat{\mathbf{v}}^{(L)(m)} = (m-1)(m-1+\alpha)\,\hat{\mathbf{v}}^{(L)(m)} \quad m=1,2,...,n-q. \tag{3.51}$$

There holds, moreover, the equation

$$\mathbf{J}\hat{\mathbf{v}}^{(L)(m)} = \delta_{q,0}(-)^{n-m}[(n-m)!\,k_n]^{-1}\,\mathbf{u}. \tag{3.52}$$

Note that only if $q=0$ is the complete spectrum of $\hat{\mathbf{N}}^{(L)}$ determined; for instance, for $n=2$ and $q=1$ the matrix $\hat{N}^{(L)}$ has, in addition to the eigenvalue 0 [corresponding to $m=1$; see (3.51)], the eigenvalue $1+\alpha-x_1-x_2$.

Also note the relation

$$\hat{\mathbf{N}}^{(L)} = \mathbf{X}[(n-1-q)\,\mathbf{I} - \mathbf{N}^{(L)}], \tag{3.53}$$

which is clearly implied by (3.20) and (3.48).

A third example is obtained from the differential equation

$$(1-x^2)\,y'' + [\beta - \alpha - (\alpha+\beta+2)\,x]\,y' - 2\,[q(q+\alpha)(1-x)^{-1} + r(r+\beta)(1+x)^{-1}]\,y + (q+r+s)(q+r+s+\alpha+\beta+1)\,y = 0,$$

$$y \equiv (1-x)^q(1+x)^r P_s^{(\alpha+2q,\beta+2r)}(x). \tag{3.54}$$

Here and below $P_p^{(\alpha,\beta)}(x)$ is the Jacobi polynomial[9,10] of degree p. It can be formulated in the following form.

Proposition 3.7: The matrix $\mathbf{N}^{(J)}$ defined by (3.30) satisfies the equation

$$[\mathbf{N}^{(J)} + 2q(q+\alpha)(\mathbf{I}-\mathbf{X})^{-1} + 2\,r(r+\beta)(\mathbf{I}+\mathbf{X})^{-1} - (q+r+s)(q+r+s+\alpha+\beta+1)] \times (\mathbf{I}-\mathbf{X})^q(\mathbf{I}+\mathbf{X})^r P_s^{(\alpha+2q,\beta+2r)}(\mathbf{X})\,\mathbf{v} = 0, \tag{3.55}$$

provided q, r, and s are three nonnegative integers whose sum is less than n,

$$q=0,1,...,n-1; \quad r=0,1,...,n-1;$$
$$s=0,1,...,n-1; \quad q+r+s<n, \tag{3.56}$$

and the (otherwise arbitrary) n different numbers x_j satisfy the restrictions

$$x_j \neq 1, \quad j=1,2,...,n, \quad \text{if} \quad q\neq 0, \tag{3.57a}$$

$$x_j \neq -1, \quad j=1,2,...,n, \quad \text{if} \quad r\neq 0. \tag{3.57b}$$

Immediate consequences of this Proposition are the following two Corollaries (in addition to Proposition 3.4).

Corollary 3.7.1: The matrix of order n

$$\tilde{\mathbf{N}}^{(J)} = \mathbf{N}^{(J)} + 2q(q+\alpha)(\mathbf{I}-\mathbf{X})^{-1} + 2r(r+\beta)(\mathbf{I}+\mathbf{X})^{-1}, \tag{3.58}$$

with $\mathbf{N}^{(J)}$ defined by (3.30), $\mathbf{I}$ the unit matrix, α and β arbitrary, q and r nonnegative integers whose sum is less than n,

$$q=0,1,...,n-1; \quad r=0,1,...,n-1; \quad q+r<n, \tag{3.59}$$

and the matrix $\mathbf{X}$ defined by (1.7) in terms of the n different numbers x_j, arbitrary except for the restrictions

$$x_j \neq 1, \quad j=1,2,...,n, \quad \text{if} \quad q\neq 0, \tag{3.60a}$$

$$x_j \neq 1, \quad j=1,2,...,n, \quad \text{if} \quad r\neq 0, \tag{3.60b}$$

has the $n-q-r$ eigenvalues

$(q+r+m-1)(q+r+m+\alpha+\beta)$

$m=1,2,...,n-q-r$, and the corresponding eigenvectors are

$$\tilde{\mathbf{v}}^{(J)(m)} = (\mathbf{I}-\mathbf{X})^q(\mathbf{I}+\mathbf{X})^r P_{m-1}^{(\alpha+2q,\beta+2r)}(\mathbf{X})\,\mathbf{v}, \quad m=1,2,...,n-q-r, \tag{3.61}$$

with $P_p^{(\alpha,\beta)}(x)$ the Jacobi polynomial[9,10] of order p and $\mathbf{v}$ defined by (1.4) [with (1.2) and (1.1)]:

$$\tilde{\mathbf{N}}^{(J)}\tilde{\mathbf{v}}^{(J)(m)} = (m-1+q+r)(m+\alpha+\beta+q+r)\,\tilde{\mathbf{v}}^{(J)(m)}, \quad m=1,2,...,n-q-r. \tag{3.62}$$

There holds, moreover, the equation

$$\mathbf{J}\tilde{\mathbf{v}}_{(J)(m)} = \delta_{m,n-q-r}(-)^q 2^{l-m} \times \binom{2(m-1)+\alpha+\beta}{m-1} k_n^{-1}\mathbf{u}. \tag{3.63}$$

Note the property of invariance under the transformation $\mathbf{X} \longleftrightarrow -\mathbf{X}$ (implying $\mathbf{Z} \longleftrightarrow -\mathbf{Z}$), $\alpha \longleftrightarrow \beta$, $q \longleftrightarrow r$; and the fact that the eigenvalues (given by this Corollary) depend on the two numbers α and β only through their sum, and on the two integers q and r also only through their sum. The complete spectrum of $\tilde{\mathbf{N}}^{(J)}$ is given only if $q = r = 0$ (in which case this Corollary reduces to Proposition 3.4); for instance, for $n = 2$, $q = 1$, and $r = 0$ the matrix $\tilde{\mathbf{N}}^{(J)}$ has, in addition to the eigenvalue $2 + \alpha + \beta$ [corresponding to $m = 1$; see (3.62)], the eigenvalue $2(1 + \alpha)[(1 - x_1)^{-1} + (1 - x_2)^{-1}]$.

Corollary 3.7.2: The matrix of order n

$$\hat{\mathbf{N}}^{(J)} = (\mathbf{X} - \mathbf{I})\,\mathbf{N}^{(J)} + (n - 1 - q)(n - q + \alpha + \beta)\,\mathbf{X} - 4r(r + \beta)(\mathbf{I} + \mathbf{X})^{-1}, \tag{3.64}$$

where $\mathbf{I}$ is the unit matrix, $\mathbf{X}$ is defined by (1.7) in terms of the n different numbers x_j, arbitrary except for the requirement

$$x_j \neq 1, \quad j = 1,2,\ldots,n \quad \text{if} \quad r \neq 0, \tag{3.65}$$

α and β are arbitrary, q and r are two nonnegative integers whose sum is less than n,

$$q = 0,1,\ldots,n-1; \quad r = 0,1,\ldots,n-1; \quad q + r < n, \tag{3.66}$$

and $\mathbf{N}^{(J)}$ is defined by (3.30), has the $n - q - r$ eigenvalues $2(m-1)(m-1+\alpha) - (n-1-q)(n-q+\alpha+\beta) - 2r(r+\beta)$, $m = 1,2,\ldots,n-q-r$, and the corresponding eigenvectors are

$$\hat{\mathbf{v}}^{(J)(m)} = (\mathbf{I} - \mathbf{X})^{m-1}(\mathbf{I} + \mathbf{X})^r P_{n-m-q-r}^{(\alpha+2m,\beta+2r)}(\mathbf{X})\,\mathbf{v}, \quad m = 1,2,\ldots,n-q-r, \tag{3.67}$$

where $P_p^{(\alpha,\beta)}(x)$ is the Jacobi polynomial[9,10] of order p and $\mathbf{v}$ is defined by (1.4) [with (1.2) and (1.1)]:

$$\hat{\mathbf{N}}^{(J)}\,\hat{\mathbf{v}}^{(J)(m)} = [2(m-1)(m-1+\alpha) - (n-1-q)(n-q+\alpha+\beta) - 2r(r+\beta)]\,\hat{\mathbf{v}}^{(J)(m)}, \quad m = 1,2,\ldots,n-q-r. \tag{3.68}$$

There holds, moreover, the equation

$$\mathbf{J}\hat{\mathbf{v}}^{(J)(m)} = \delta_{q,0}(-)^{m-1}2^{m+r-n} \times \binom{2(n-m-r)+\alpha+\beta}{n-m-r} k_n^{-1}\,\mathbf{u}. \tag{3.69}$$

Note that the complete spectrum is given only if $q = r = 0$; for instance, for $n = 2$, $q = 1$, $r = 0$, the eigenvalues are 0 [corresponding to $m = 1$; see (3.68)] and $-2(1+\beta) + (\alpha+\beta+2)(x_1 + x_2)$, and for $n = 2$, $q = 0$, $r = 1$ the eigenvalues are $-(\alpha + 3\beta + 4)$ [corresponding to $m = 1$; see (3.68)] and $\alpha + \beta + 2 + x_1 + x_2 - 4(1+\beta) \times [(1+x_1)^{-1} + (1+x_2)^{-1}]$.

We end this section emphasizing two points, that are relevant in view of possible applications of these results to test computer programs. (i) All the matrices we have given have a completely explicit representation; in particular, no matrix products are involved, or matrix inversions, except with diagonal matrices. (ii) It is clearly posssible to construct in this way an enormous variety of test matrices with *a priori* known eigenvalues, including matrices having only a few very large off-diagonal elements.

4. PROPERTIES OF CERTAIN MATRICES CONSTRUCTED WITH THE ZEROS OF SPECIAL POLYNOMIALS

In this section we consider properties analogous to those discussed in Sec. 3, but now for matrices constructed, rather than with n arbitrary numbers, with the zeros of special polynomials. It is then generally possible to compute in closed form the sums that enter in the definitions, (1.10) and (1.17), of the matrices $\mathbf{Z}$ and $\mathbf{Z}^2$, thereby obtaining more explicit representations of these matrices. Moreover, additional results, in addition to those of Secs. 1 and 3 (which continue, of course, to hold), can be obtained.

In Subsec. 4.1 we consider the (very simple) case in which the numbers x_j are the n roots of unity. This choice yields, among other results, certain novel representations of the classical polynomials.

In the subsequent subsections we consider the cases in which the numbers x_j are the zeros of the classical polynomials. These choices reproduces, among other results, those of Ref. 3.

4.1. Matrices constructed with the roots of unity

In this subsection we take the following specific choice for the polynomials (1.1):

$$p_n(x) = (x^n - 1)/n, \tag{4.1.1}$$

implying, of course,

$$p_n'(x) = x^{n-1}. \tag{4.1.2}$$

This choice implies (in the notation of Sec. 1):

$$x_j = \exp(2\pi i j/n), \quad j = 1,2,\ldots,n, \tag{4.1.3}$$

$$\xi_j = \tfrac{1}{2}(n-1)/x_j, \quad j = 1,2,\ldots,n, \tag{4.1.4a}$$

$$\xi_j^{(2)} = \tfrac{1}{12}(n-1)(5-n)/x_j^2, \quad j = 1 = 1,2,\ldots,n, \tag{4.1.4b}$$

$$v_j = x_j, \quad j = 1,2,\ldots,n. \tag{4.1.5}$$

To obtain (4.1.4) we have used the identities

$$\sum_{l=1}^{n}{}' \{1 - \exp[2\pi i(l-j)/n]\}^{-1} = \tfrac{1}{2}(n-1), \tag{4.1.6a}$$

$$\sum_{l=1}^{n} \{1 - \exp[2\pi i(l-j)/n]\}^{-2} = \tfrac{1}{12}(n-1)(5-n), \tag{4.1.6b}$$

whose proof is reported in Appendix B.

Equations (4.1.4) are the formulas that provide the more explicit representations of the matrices $\mathbf{Z}$ and $\mathbf{Z}^2$ mentioned in the introduction to this section. A number of explicit matrices can now be constructed, whose matrix elements are elementary functions of rational angles, and whose spectrum and eigenvectors are known. They are obtained, of course, by inserting in the results of Sec. 3 the special choice (4.1.3) [implying (4.1.4,5)]. In particular, it is easily seen that the results of Proposition 3.1 reproduce Theorem 1 of Ref. 11, the matrix

$$A_{jk} = (1 - \delta_{jk})\{1 + i\cot[(j-k)\pi/n]\}, \tag{4.1.7a}$$

[see Eq. (1) of Ref. 11] being related to the matrix $\mathbf{N}$ of (3.6) [with (4.1.3)] by

$$\mathbf{A} = (n-1)\,\mathbf{I} - 2\mathbf{X}^{-1}\mathbf{N}\mathbf{X}. \tag{4.1.7b}$$

It is left to the diligent reader to write in explicit detail all the "diophantine relations involving functions of rational angles" [11] that can be easily obtained in this manner.

In the rest of this subsection we focus on the results of Proposition 3.1, that still read

$$\mathbf{N}\mathbf{v}^{(m)} = (m-1)\,\mathbf{v}^{(m)}, \quad m = 1,2,\dots,n, \tag{4.1.8}$$

$$\mathbf{Z}\mathbf{v}^{(m)} = (m-1)\,\mathbf{v}^{(m-1)}, \quad m = 1,2,\dots,n, \tag{4.1.9}$$

$$\mathbf{X}\mathbf{v}^{(m)} = \mathbf{v}^{(m+1)} \quad m = 1,2,\dots,n-1, \tag{4.1.10}$$

$$\mathbf{J}\mathbf{v}^{(m)} = \delta_{mn}\, n\mathbf{u}, \quad m = 1,2,\dots,n, \tag{4.1.11}$$

but now with

$$N_{jk} = \tfrac{1}{2}(n-1)\,\delta_{jk} + (1-\delta_{jk})\,x_j/(x_j - x_k), \tag{4.1.12a}$$

$$N_{jk} = \tfrac{1}{2}(n-1)\delta_{jk} + (1-\delta_{jk})\{1 - \exp[2\pi i(k-j)/n]\}^{-1}, \tag{4.1.12b}$$

$$Z_{jk} = \tfrac{1}{2}(n-1)\,x_j^{-1}\,\delta_{jk} + (1-\delta_{jk})(x_j - x_k)^{-1}, \tag{4.1.13}$$

$$v_j^{(m)} = x_j^m = \exp(2\pi i\, jm/n). \tag{4.1.14}$$

The last formula, together with (4.1.3) and (1.3), implies

$$\mathbf{v}^{(n)} = \mathbf{u}, \tag{4.1.15}$$

and therefore (4.1.10) and (4.1.11) imply

$$\mathbf{X}(\mathbf{I} - \mathbf{J}/n)\mathbf{v}^{(m)} = (1-\delta_{mn})\mathbf{v}^{(m+1)}, \quad m = 1,2,\dots,n. \tag{4.1.16}$$

Thus the matrices

$$\mathbf{A}^{(-)} = \mathbf{Z}, \quad \mathbf{A}^{(+)} = \mathbf{X}(\mathbf{I} - \mathbf{J}/n), \tag{4.1.17}$$

act on the eigenvectors $\mathbf{v}^{(m)}$ as lowering and raising operators,

$$\mathbf{A}^{(-)}\mathbf{v}^{(m)} = (m-1)\mathbf{v}^{(m-1)}, \quad m = 1,2,\dots,n, \tag{4.1.18a}$$

$$\mathbf{A}^{(+)}\mathbf{v}^{(m)} = (1-\delta_{mn})\mathbf{v}^{(m+1)}, \quad m = 1,2,\dots,n. \tag{4.1.18b}$$

Actually, the property of acting as a lowering operator is possessed by the operator $\mathbf{Z}$ independently of the special choice of the x_j's considered here, see (3.9) or (4.1.9); and the property of acting as a raising operator is also possessed generally by $\mathbf{X}$, see (3.10) or (4.1.10), except, however, for the highest eigenvector, that should be annihilated by a proper raising operator acting in a finite dimensional space: a property possessed by $\mathbf{A}^{(+)}$, with the special choice of x_j's discussed in this subsection, but not, generally, by $\mathbf{X}$. The importance of this will be immediately apparent. Note that Eqs. (4.1.18) imply that $\mathbf{A}^{(-)}$ and $\mathbf{A}^{(+)}$ are nilpotent:

$$\mathbf{A}^{(-)n} = 0, \quad \mathbf{A}^{(+)n} = 0. \tag{4.1.19}$$

The first of these equations is, of course, merely a special case of (1.25). It is, moreover, easily seen that the three matrices $\mathbf{A}^{(-)}$, $\mathbf{A}^{(+)}$, and $\mathbf{N}$ satisfy the standard commutation rules

$$[\mathbf{A}^{(\mp)},\mathbf{N}] = \pm\mathbf{A}^{(\mp)}, \tag{4.1.20}$$

and are related by

$$\mathbf{A}^{(+)}\mathbf{A}^{(-)} = \mathbf{N}, \tag{4.1.21a}$$

$$\mathbf{A}^{(-)}\mathbf{A}^{(+)} = \mathbf{N} + \mathbf{I} - \mathbf{J}, \tag{4.1.21b}$$

implying, of course,

$$[\mathbf{A}^{(-)},\mathbf{A}^{(+)}] = \mathbf{I} - \mathbf{J}. \tag{4.1.21c}$$

Moreover,

$$\mathbf{J}\mathbf{N} = \mathbf{N}\mathbf{J} = (n-1)\mathbf{J}, \tag{4.1.22}$$

implying, of course,

$$[\mathbf{J},\mathbf{N}] = 0. \tag{4.1.23}$$

Note that the matrix $\mathbf{N}$ is now Hermitian, see (4.1.12b), and this implies that its eigenvectors are orthogonal, as can be easily verified:

$$(\mathbf{v}^{(l)},\mathbf{v}^{(m)}) = \sum_{j=1}^{n} v_j^{(l)*} v_j^{(m)} = n\delta_{lm}. \tag{4.1.24}$$

We now follow the reasoning of Ref. 6. We thus get the following Lemma.

Lemma 4.4.1: The eigenvalues μ of the generalized eigenvalue equation

$$\mathbf{M}^{(1)}(\theta)\mathbf{v}(\theta) = \mu\mathbf{M}^{(2)}(\theta)\mathbf{v}(\theta), \tag{4.1.25}$$

where the two matrices $\mathbf{M}^{(1)}(\theta)$ and $\mathbf{M}^{(2)}(\theta)$, of order n, are defined by

$$\mathbf{M}^{(s)}(\theta) = \sum_{p=0}^{\infty}\sum_{q=0}^{n-1}\sum_{r=0}^{n-1} c_{pqr}^{(s)} \exp[i(r-q)\theta]\times[\mathbf{A}^{(-)}]^q[\mathbf{A}^{(+)}]^r\ \mathbf{N}^p, \quad s = 1,2, \tag{4.1.26}$$

with $\mathbf{N}$ and $\mathbf{A}^{(\pm)}$ defined by (4.1.12), (4.1.17), (4.1.13), (1.7), and (4.1.3), and the coefficients $c_{pqr}^{(s)}$ arbitrary (but independent of θ)], are independent of θ; indeed they coincide with the eigenvalues of the (θ-independent) generalized eigenvalue equation

$$\mathbf{R}^{(1)}\mathbf{a} = \mu\mathbf{R}^{(2)}\mathbf{a}, \tag{4.1.27}$$

where the matrices $\mathbf{R}^{(1)}$ and $\mathbf{R}^{(2)}$, of order n, are defined by

$$R_{lm}^{(s)} = [(l-1)!]^{-1}\sum_{p=0}^{\infty}(m-1)^p \times\sum_{q=q_{\min}}^{n-l} c_{p,q,l+q-m}^{(s)}(l+q-1)! \tag{4.1.28}$$

$$q_{\min} = \max(0,m-l). \tag{4.1.29}$$

Proof: Set, in (4.1.25),

$$\mathbf{v}(\theta) = \sum_{m=1}^{n} a_m \exp(im\theta)\mathbf{v}^{(m)}, \tag{4.1.30}$$

and using (4.1.18), (4.1.8), and (4.1.24) obtain (4.1.27) [of course the coefficients a_m in (4.1.30) are the components of the vector $\mathbf{a}$ in (4.1.27)]. Q.E.D.

We are, of course, assuming the coefficients $c_{pqr}^{(s)}$ vanish sufficiently fast as $p\rightarrow\infty$ to exclude any convergence problem in (4.1.26) and (4.1.28). Note that the commutation relations (4.1.20), together with (4.1.21a), imply that no additional generality would be implied by the inclusion of additional terms in the rhs of (4.1.26) differing from those now present in the ordering of the matrices $\mathbf{A}^{(-)}$, $\mathbf{A}^{(+)}$, and $\mathbf{N}$.

It is of interest to consider special cases of this Lemma. The idea is to induce, by an appropriate choice of the coefficients $c_{pqr}^{(s)}$, the Eq. (4.1.28) to reproduce the recursion relations of the classical polynomials—a very easy task.

The first choice we consider is the case with all but three of the coefficients $c_{pqr}^{(s)}$ vanishing:

$$c_{010}^{(1)} = c_{001}^{(1)} = 2^{-1/2}, \quad c_{000}^{(2)} = 1,$$
$$c_{pqr}^{(s)} = 0 \quad \text{otherwise}. \tag{4.1.31}$$

It is then easily seen that (4.1.27) becomes

$$ma_{m+1} + a_{m-1} = 2^{1/2}\mu a_m ,$$
$$a_m = 0, \quad \text{if} \quad m \leqslant 0 \text{ or } m > n, \tag{4.1.32}$$

yielding

$$a_m = H_{m-1}(\mu)/[2^{m/2}(m-1)!], \quad m = 1,2,...,n, \tag{4.1.33}$$

with the eigenvalue condition

$$H_n(\mu) = 0, \tag{4.1.34}$$

where $H_p(x)$ is the Hermite polynomial[9,10] of degree p. This implies the following results.

Proposition 4.1.1: The n eigenvalues of the matrix of order n

$$\mathbf{M}^{(H)}(\theta) = 2^{-1/2}[\mathbf{A}^{(-)}\exp(-i\theta) + \mathbf{A}^{(+)}\exp(i\theta)], \tag{4.1.35}$$

with θ arbitrary and $\mathbf{A}^{(\pm)}$ defined by (4.1.17), (4.1.13), (1.7), (1.6), and (4.1.3), coincide with the n zeros of the Hermite polynomial of order n, and the corresponding (unnormalized) eigenvectors are given by the formula

$$\mathbf{v}^{(H)(j)}(\theta) = \sum_{m=1}^{n} [2^{m/2}(m-1)!]^{-1} H_{m-1}(x_j^{(n)}) \times \exp(im\theta)\mathbf{v}^{(m)}, \tag{4.1.36}$$

where the vectors $\mathbf{v}^{(m)}$ are defined by (4.1.14) and $x_j^{(n)}$ is the jth zero of the Hermite polynomial of order n:

$$H_n(x_j^{(n)}) = 0, \quad j = 1,2,...,n, \tag{4.1.37}$$
$$\mathbf{M}^{(H)}(\theta)\mathbf{v}^{(H)(j)}(\theta) = x_j^{(n)}\mathbf{v}^{(H)(j)}(\theta), \quad j = 1,2,...,n. \tag{4.1.38}$$

Corollary 4.1.1.1: There holds for Hermite polynomials[9,10] the representation

$$H_n(x) = 2^n \det[x\mathbf{I} - \mathbf{M}^{(H)}(\theta)], \tag{4.1.39}$$

where $\mathbf{I}$ is the unit matrix of order n, θ is arbitrary and the matrix $\mathbf{M}^{(H)}(\theta)$ is defined by (4.1.35).

Completely equivalent, but slightly neater, formulas are obtained by replacing $M(\theta)$ in (4.1.35) and/or in (4.1.39) by

$$H(\varphi) = M^{(H)}(\theta), \tag{4.1.40}$$

with

$$\exp(2i\theta) \equiv n \exp(4i\varphi). \tag{4.1.41}$$

The explicit form of $H(\varphi)$ is displayed by (I.7).

We now give without further comments the analogous results for Laguerre and Jacobi polynomials. The latter will be preceded by the display of the (special) cases of Legendre and Gegenbauer (or ultraspherical) polynomials, which entail considerable simplifications.

Proposition 4.1.2: The n eigenvalues of the matrix of order n

$$\mathbf{M}^{(L)}(\theta) = (1+\alpha)\mathbf{I} + 2\mathbf{N} - \mathbf{A}^{(-)}\exp(-i\theta) - \mathbf{A}^{(+)}[(1+\alpha)\mathbf{I} + \mathbf{N}]\exp(i\theta), \tag{4.1.42}$$

with θ and α arbitrary, $\mathbf{I}$ the unit matrix and $\mathbf{A}^{(\pm)}$ and $\mathbf{N}$ defined by (4.1.17), (4.1.13), (4.1.12), (1.7), (1.6), and (4.1.3), coincide with the n zeros of the (generalized) Laguerre polynomial $L_n^{\alpha}(x)$,[10] and the corresponding (unnormalized) eigenvectors are given by the formula

$$\mathbf{v}^{(L)(j)}(\theta) = \sum_{m=1}^{n} L_{m-1}^{\alpha}(y_j^{(n)}(\alpha))\exp(im\theta)\mathbf{v}^{(m)}, \tag{4.1.43}$$

where the vectors $\mathbf{v}^{(m)}$ are defined by (4.1.14) and $y_j^{(n)}(\alpha)$ is the jth zero of the (generalized) Laguerre polynomial of order n:

$$L_n^{\alpha}[y_j^{(n)}(\alpha)] = 0, \quad j = 1,2,...,n, \tag{4.1.44}$$
$$\mathbf{M}^{(L)}(\theta)\mathbf{v}^{(L)(j)}(\theta) = y_j^{(n)}(\alpha)\mathbf{v}^{(L)(j)}(\theta), \quad j = 1,2,...,n \tag{4.1.45}$$

Corollary 4.1.2.1: There holds for (generalized) Laguerre polynomials[10] the representation

$$L_n^{(\alpha)}(x) = (n!)^{-1}\det[\mathbf{M}^{(L)}(\theta) - x\mathbf{I}], \tag{4.1.46}$$

where $\mathbf{I}$ is the unit matrix, θ is arbitrary and $\mathbf{M}^{(L)}(\theta)$ is defined by (4.1.42).

Completely equivalent, but perhaps slightly neater, formulas are obtained by replacing $\mathbf{M}^{(L)}(\theta)$ by $\mathbf{L}(a)$ in (4.1.42) (4.1.45) and/or (4.1.46), with a arbitrary and $\mathbf{L}(a)$ explicitly defined by

$$L_{jk}(a) = \delta_{jk}\{\alpha + n - \tfrac{1}{2}[(n-1)(2\alpha+n)/n](x_j/a) - \tfrac{1}{2}(n-1)(a/x_j)\} + (1-\delta_{jk})\{[(\alpha+n)/n] \times (x_j/a) - (x_j - a)^2/[a(x_j - x_k)]\}, \tag{4.1.47}$$

with the x_j's defined of course by (4.1.3). Note that this matrix $\mathbf{L}(a)$ has nothing to do with the matrix $\mathbf{L}(\theta)$ of (I.4); its relation to $\mathbf{M}^{(L)}(\theta)$, (4.1.42), is given simply by

$$\mathbf{M}(\theta) = \mathbf{L}[\exp(-i\theta)]. \tag{4.1.48}$$

Proposition 4.1.3: The n eigenvalues μ of the generalized eigenvalue equation (4.1.25) with

$$\mathbf{M}^{(P)(1)}(\theta) = \mathbf{A}^{(-)}\exp(-i\theta) + \mathbf{N}\mathbf{A}^{+}, \tag{4.1.49a}$$
$$\mathbf{M}^{(P)(2)}(\theta) = \mathbf{M}^{(P)(2)} = \mathbf{I} + 2\,\mathbf{N}, \tag{4.1.49b}$$

[where θ is arbitrary, $\mathbf{I}$ is the unit matrix of order n, and the three matrices $\mathbf{A}^{(\pm)}$ and $\mathbf{N}$, of order n, are defined by (4.1.17), (4.1.12), (1.7), (1.6), and (4.1.3)] coincide with the n zeros of the Legendre polynomial $P_n(x)$,[9,10] and the corresponding (unnormalized) eigenvectors are given by the formula

$$\mathbf{v}^{(P)(j)}(\theta) = \sum_{m=1}^{n} P_{m-1}(z_j^{(m)})\exp(im\theta)\mathbf{v}^{(m)}, \tag{4.1.50}$$

where the vectors $\mathbf{v}^{(m)}$ are defined by (4.1.14) and $z_j^{(n)}$ is the jth zero of the Legendre polynomial of order n:

$$P_n(z_j^{(n)}) = 0, \quad j = 1,2,...,n, \tag{4.1.51}$$
$$\mathbf{M}^{(P)(1)}(\theta)\mathbf{v}^{(P)(j)}(\theta) = z_j^{(n)}\mathbf{M}^{(P)(2)}\mathbf{v}^{(P)(j)}(\theta). \tag{4.1.52}$$

Corollary 4.1.3.1: There holds for Legendre polynomials[9,10] the representation

$$P_n(x) = \det[\mathbf{M}^{(P)(1)}(\theta) - x\mathbf{M}^{(P)(2)}]/\det[\mathbf{M}^{(P)(1)}(\theta) - \mathbf{M}^{(P)(2)}], \tag{4.1.53}$$

where θ is arbitrary and the two matrices $\mathbf{M}^{(P)(1)}(\theta)$ and $\mathbf{M}^{(P)(2)}$, of order n, are defined by (4.1.49).

Proposition 4.1.4: The n eigenvalues μ of the generalized eigenvalue equation (4.1.25) with

$$\mathbf{M}^{(C)(1)}(\theta) = (\mathbf{N} + 2\lambda\,\mathbf{I})\mathbf{A}^{(-)}\exp(-i\theta) + [(\mathbf{N} + \lambda\,\mathbf{I})^2 - \tfrac{1}{4}\mathbf{I}]\mathbf{A}^{(+)}\exp(i\theta), \tag{4.1.54a}$$

$$\mathbf{M}^{(C)(2)}(\theta) = \mathbf{M}^{(C)(2)} = 2(\mathbf{N} + \lambda\,\mathbf{I})[\mathbf{N} + (\lambda + \tfrac{1}{2})\mathbf{I}] \qquad (4.1.54b)$$

[where θ and λ are arbitrary, $\mathbf{I}$ is the unit matrix of order n, and the 3 matrices $\mathbf{A}^{(\pm)}$ and $\mathbf{N}$, of order n, are defined by (4.1.17), (4.1.12), (1.7), (1.6), and (4.1.3)], coincide with the n zeros of the Gegenbauer polynomial $C_n(x)$,[10] and the corresponding (unnormalized) eigenvectors are given by the formula

$$\mathbf{v}^{(C)(j)}(\theta) = \sum_{m=1}^{n} \left(\frac{\Gamma(m+\lambda-\frac{1}{2})}{\Gamma(m+2\lambda-1)} \right) C^{\lambda}_{m-1}\,[z_j^{(n)}(\lambda)] \times \exp(im\theta)\mathbf{v}^{(m)}, \qquad (4.1.55)$$

where the vectors $\mathbf{v}^{(m)}$ are defined by (4.1.14) and $z_j^{(n)}(\lambda)$ is the jth zero of the Gengenbauer polynomial of order n:

$$C^{\lambda}_{n}[z_j^{(n)}(\lambda)] = 0, \quad j = 1,2,...,n, \qquad (4.1.56)$$

$$\mathbf{M}^{(C)(1)}(\theta)\mathbf{v}^{(C)(j)}(\theta) = z_j^{(n)}(\lambda)\mathbf{M}^{(C)(2)}\mathbf{v}^{(C)(j)}(\theta), \quad j = 1,2,...,n. \qquad (4.1.57)$$

Corollary 4.1.4.1: There holds for Gegenbauer polynomials[10] the representation

$$C^{\lambda}_{n}(x) = \binom{n+2\lambda-1}{n} \frac{\det[\mathbf{M}^{(C)(1)}(\theta) - x\mathbf{M}^{(C)(2)}]}{\det[\mathbf{M}^{(C)(1)}(\theta) - \mathbf{M}^{(C)(2)}]}, \qquad (4.1.58)$$

where θ is arbitrary and the two matrices $\mathbf{M}^{(C)(1)}(\theta)$ and $\mathbf{M}^{(C)(2)}$, of order n, are defined by (4.1.54).

Proposition 4.1.5: The n eigenvalues μ of the generalized eigenvalue equation (4.1.25) with

$$\begin{aligned}\mathbf{M}^{(J)(1)}(\theta) &= (\beta^2 - \alpha^2)[2\mathbf{N} + (\alpha+\beta+1)\mathbf{I}] + 2\mathbf{A}^{(-)} \\ &\quad \times [\mathbf{N} + (\alpha+\beta)\mathbf{I}][2\mathbf{N} + (\alpha+\beta-2)\mathbf{I}] \\ &\quad \times \exp(-i\theta) + 2(\mathbf{N} + \alpha\mathbf{I})(\mathbf{N} + \beta\mathbf{I})[2\mathbf{N} \\ &\quad + (\alpha+\beta+2)\mathbf{I}]\mathbf{A}^{(+)}\exp(i\theta), \end{aligned} \qquad (4.1.59a)$$

$$\mathbf{M}^{(J)(2)}(\theta) = \mathbf{M}^{(J)(2)} = [2\mathbf{N} + (\alpha+\beta)\mathbf{I}] \times [2\mathbf{N} + (\alpha+\beta+1)\mathbf{I}][2\mathbf{N} + (\alpha+\beta+2)\mathbf{I}], \qquad (4.1.59b)$$

[where θ, α and β are arbitrary, $\mathbf{I}$ is the unit matrix of order n and the three matrices $\mathbf{A}^{(\pm)}$ and $\mathbf{N}$, of order n, are defined by (4.1.17), (4.1.12), (1.7), (1.6), and (4.1.3)], coincide with the n zeros of the Jacobi polynomial $P_n^{(\alpha,\beta)}(x)$,[9,10] and the corresponding (unnormalized eigenvectors are given by the formula

$$\mathbf{v}^{(J)(j)}(\theta) = \sum_{m=1}^{n} P^{(\alpha,\beta)}_{m-1}\,[z_j^{(n)}(\alpha,\beta)]\exp(im\theta)\mathbf{v}^{(m)}, \qquad (4.1.60)$$

where the vectors $\mathbf{v}^{(m)}$ are defined by (4.1.14) and $z_j^{(n)}(\alpha,\beta)$ is the jth zero of the Jacobi polynomial of order n:

$$P_n^{(\alpha,\beta)}[z_j^{(n)}(\alpha,\beta)] = 0, \quad j = 1,2,...,n, \qquad (4.1.61)$$

$$\mathbf{M}^{(J)(1)}(\theta)\mathbf{v}^{(J)(j)}(\theta) = z_j^{(n)}(\alpha,\beta)\mathbf{M}^{(J)(2)}\mathbf{v}^{(J)(j)}(\theta), \quad j = 1,2,...,n. \qquad (4.1.62)$$

Corollary 4.1.5.1: There holds for Jacobi polynomials[9,10] the representation

$$P_n^{(\alpha,\beta)}(x) = \binom{n+\alpha}{n} \frac{\det[\mathbf{M}^{(J)(1)}(\theta) - x\mathbf{M}^{(J)(2)}]}{\det[\mathbf{M}^{(J)(1)}(\theta) - \mathbf{M}^{(J)(2)}]}, \qquad (4.1.63)$$

where θ, α and β are arbitrary and the two matrices $\mathbf{M}^{(J)(1)}(\theta)$ and $\mathbf{M}^{(J)(2)}$, of order n, are defined by (4.1.59).

4.2. Matrices constructed with the zeros of Hermite polynomials

In this subsection we take the following specific choice for the polynomial (1.1):

$$p_n(x) = [\pi^{1/2}2^n n!]^{-1/2}H_n(x), \qquad (4.2.1)$$

where $H_n(x)$ is the Hermite polynomial[9,10] of order n. The normalization factor has been introduced for consistency with the results of Sec. 2, that are now applicable with

$$a = -\infty, \quad b = +\infty, \quad w(x) = \exp(-x^2), \qquad k_n = [\pi^{1/2}2^n n!]^{-1/2}. \qquad (4.2.2)$$

Thus, throughout this subsection, the x_j's are the n zeros of the Hermite polynomial of order n,

$$H_n(x_j) = 0, \quad j = 1,2,...,n. \qquad (4.2.3)$$

These numbers depend, of course, on n, but this is not explicitly indicated here (for notational simplicity).

This choice yields, in the notation of Secs. 1 and 2,[3]

$$\xi_j = x_j\,, \qquad (4.2.4)$$

$$\xi_j^{(2)} = \tfrac{2}{3}(n-1) - \tfrac{1}{3}x_j^2\,, \qquad (4.2.5)$$

$$c_j = \tfrac{1}{2}, \qquad (4.2.6)$$

$$u_m^{(j)} = \{2^{n+1-m}(n-1)!/[n(m-1)!]\}^{1/2}H_{m-1}(x_j)/H_{n-1}(x_j). \qquad (4.2.7)$$

Note that (4.2.6) implies that the matrix $\mathbf{C}$ of Sec. 2, see (2.39), is now a multiple of the unit matrix $\mathbf{I}$; thus, in this case the matrices $\mathbf{Z}$ and $\tilde{\mathbf{Z}}$ coincide, see (2.38).

These equations, in particular (4.2.4) and (4.2.5), can be combined with the results of Sec. 3. Particularly neat results are obtained from those of Proposition 3.2, in view of the vanishing of the rhs of (3.18b) implied by (4.2.3); the corresponding formulas also match neatly the results of Ref. 3 (see in particular Proposition 3.3 of that paper) via the relation

$$\mathbf{N}^{(H)} = (n-1)\mathbf{I} - \mathbf{A}, \qquad (4.2.8)$$

with $\mathbf{A}$ defined by (I.1) and $\mathbf{N}^{(H)}$ by (3.14).

It is, moreover, convenient to define the two matrices $\mathbf{A}^{(\pm)}$, the three differential operators $\mathcal{A}^{(\pm)}$ and $\mathcal{A}$, and the three quantities $\alpha_m^{(\pm)}$ and a_m as follows:

$$\mathbf{A}^{(-)} = \mathbf{Z}, \quad \mathbf{A}^{(+)} = 2\mathbf{X} - \mathbf{Z}, \qquad (4.2.9a)$$

$$A_{jk}^{(\pm)} = \delta_{jk}x_j \mp (1-\delta_{jk})(x_j - x_k)^{-1}, \qquad (4.2.9b)$$

$$\mathcal{A}^{(-)} = d/dx, \quad \mathcal{A}^{(+)} = 2x - d/dx, \qquad (4.2.10)$$

$$\mathcal{A} = n - 1 - \tfrac{1}{2}\mathcal{A}^{(+)}\mathcal{A}^{(-)}, \qquad (4.2.11)$$

$$\alpha_m^{(-)} = [2(m-1)]^{1/2}, \quad \alpha_m^{(+)} = (2m)^{1/2}, \quad m = 1,2,...,n, \qquad (4.2.12)$$

$$a_m = n - 1 - \tfrac{1}{2}\alpha_{m-1}^{(+)}\alpha_m^{(-)} = n - m, \quad m = 1,2,...,n. \qquad (4.2.13)$$

This guarantees, also notationally, consistency with the results of Sec. 2, and, up to trivial notational changes, with the results of Refs. 4–6 [note, however, that Eqs. (11) of Ref. 6 are misprinted, while Eqs. (10) are correct; this accounts for the inconsistency of (11) with (4.2.12)]. Note that the results of Sec. 2 go somewhat beyond those previously obtained, by displaying the explicit connection [see (4.2.7)] between the algebraic results in the n-dimensional vector space and the differential and integral properties of Hermite polynomials (indeed, all the results reported in this paper have emerged as by-products of a research originally intended merely to clarify this connection).

It is, of course, also possible to combine the special choice of x_j's considered in this subsection with other results of Sec. 3. For instance, Proposition 3.1 implies that the matrix

$$N_{jk} = \delta_{jk} x_j^2 + (1-\delta_{jk}) x_j/(x_j - x_k), \qquad (4.2.14)$$

has the first n nonnegative integers as eigenvalues; Proposition 3.5 implies that the matrix

$$\widetilde{N}_{jk}^{(H)} = \delta_{jk} [\tfrac{1}{3} x_j^2 + \tfrac{1}{3}(n-1) - \tfrac{1}{2} q(q+1) x_j^{-2}] + (1-\delta_{jk})[q x_j^{-1}(x_j - x_k)^{-1} + (x_j - x_k)^{-2}], \qquad (4.2.15a)$$

$$\widetilde{N}_{jk}^{(H)} = (n-1)\delta_{jk} - A_{jk} - \tfrac{1}{2} q(q+1)\delta_{jk} x_j^{-2} + q(1-\delta_{jk}) x_j^{-1}(x_j - x_k)^{-1} \qquad (4.2.15b)$$

[with n even (so that $x_j \neq 0, j = 1,2,...,n$) and q any nonnegative integer less than n], has the first $n - q$ integers as eigenvalues, and so on. These results are obtained easily using (4.2.4), (4.2.5), (1.10), and (1.17); the first of them is not new.[3]

The same type of reasoning[6] used in the last part of the preceding subsection can also be repeated here. It is easier to work with the (unnormalized) eigenvectors (3.15) rather than with the (normalized) eigenvectors defined by (4.2.7) and (2.23), namely, using the formulas

$$\mathbf{N}^{(H)}\mathbf{v}^{(H)(m)} = (m-1)\mathbf{v}^{(H)(m)}, \quad m = 1,2,...,n, \qquad (4.2.16)$$

$$\mathbf{A}^{(-)}\mathbf{v}^{(H)(m)} = 2(m-1)\mathbf{v}^{(H)(m-1)}, \quad m = 1,2,...,n, \qquad (4.2.17)$$

$$\mathbf{A}^{(+)}\mathbf{v}^{(H)(m)} = (1-\delta_{mn})\mathbf{v}^{(H)(m+1)}, \quad m = 1,2,...,n. \qquad (4.2.18)$$

Here, of course, $\mathbf{N}^{(H)}$ is defined by (3.14), $\mathbf{A}^{(\pm)}$ by (4.2.9), and $\mathbf{v}^{(H)(m)}$ by (3.15); but with the x_j's being now the n zeros of $H_n(x)$ [see (4.2.3), (4.2.4), and (4.2.5)]. These equations coincide essentially with (3.16)–(3.18); but note the difference between (3.18) and (4.2.18).

In complete analogy to Lemma 4.1.1, there holds now the following Lemma.

Lemma 4.2.1: The eigenvalues μ of the generalized eigenvalue equation

$$\mathbf{M}^{(1)}(\theta)\mathbf{v}(\theta) = \mu \mathbf{M}^{(2)}(\theta)\mathbf{v}(\theta), \qquad (4.2.19)$$

are independent of θ, if the two matrices $\mathbf{M}^{(1)}(\theta)$ and $\mathbf{M}^{(2)}(\theta)$, of order n, are defined by

$$\mathbf{M}^{(1)}(\theta) = \sum_{p=0}^{\infty}\sum_{q=0}^{n-1}\sum_{r=0}^{n-1} c_{pqr}^{(s)} \exp[i(r-q)\theta] \times [\mathbf{A}^{(-)}]^q [\mathbf{A}^{(+)}]^r [\mathbf{N}^{(H)}]^p, \quad s = 1,2, \qquad (4.2.20)$$

with $\mathbf{N}^{(H)}$ and $\mathbf{A}^{(\pm)}$ defined by (3.14), (4.2.9), (1.7), (1.10), (1.17), (4.2.3)–(4.2.5), and the coefficients $c_{pqr}^{(s)}$ arbitrary (but independent of θ).

The proof is too similar to that of Lemma 4.1.1 to need reporting. Moreover, again in close analogy to the results of the previous subsection, it is possible to obtain in this manner novel representations of the classical polynomials. An example of such results (whose proof can essentially be found in the literature, see Refs. 3 and 6) has been already reported in the Introduction, see (I.5). We conclude this subsection reporting two more such instances, namely, the representations of *Laguerre* and *Legendre* polynomials that one obtains in this manner, in terms of determinants of matrices of order n constructed with the n zeros of the *Hermite* polynomial $H_n(x)$. The proof of these results, as well as the derivation of analogous formulas for Gegenbauer and Jacobi polynomials, is left as an exercise for the diligent reader (and also the derivation of analogous representations of the classical polynomials—or, for that matter, any polynomials defined by simple recurrence relations—in terms of the zeros of Laguerre or Jacobi polynomials, on the basis of the results of the following Subsecs. 4.4 and 4.5).

Proposition 4.2.1: There hold for Laguerre[10] and Legendre[9,10] polynomials the representations

$$L_n^{\alpha}(x) = (n!)^{-1} \det[\mathbf{M}(\theta) - x\mathbf{I}], \qquad (4.2.21)$$

$$P_n(x) = \det[\mathbf{M}^{(1)}(\theta) - x\mathbf{M}^{(2)}]/\det[\mathbf{M}^{(1)}(\theta) - \mathbf{M}^{(2)}], \qquad (4.2.22)$$

where $\mathbf{I}$ is the unit matrix (of order n) and the three matrices $\mathbf{M}(\theta)$, $\mathbf{M}^{(1)}(\theta)$, and $\mathbf{M}^{(2)}$, of order n, are defined by

$$\mathbf{M}(\theta) = -\tfrac{1}{2}\mathbf{A}^{(-)}\exp(-i\theta) + (1+\alpha)\mathbf{I} + 2\mathbf{N}^{(H)} - (\alpha\mathbf{I} + \mathbf{N}^{(H)})\mathbf{A}^{(+)}\exp(i\theta), \qquad (4.2.23)$$

$$\mathbf{M}^{(1)}(\theta) = \mathbf{A}^{(-)}\exp(-i\theta) + 2\mathbf{N}^{(H)}\mathbf{A}^{(+)}\exp(i\theta), \qquad (4.2.24)$$

$$\mathbf{M}^{(2)} = 2(\mathbf{I} + 2\mathbf{N}^{(H)}). \qquad (4.2.25)$$

Here θ is arbitrary, while the three matrices $\mathbf{N}^{(H)}$ and $\mathbf{A}^{(\pm)}$, of order n, are defined by (3.14), (4.2.9), (1.7), (1.10), (1.17), and (4.2.3)–(4.2.5).

4.3. Matrices constructed with the zeros of combinations of Hermite polynomials

This subsection is merely to indicate, by a single example, the range of possibilities implied by the results of Sec. 3. Take for instance, for the polynomial (1.1), the choice

$$p_n(x) = H_n(x) + 2nH_{n-2}(x), \qquad (4.3.1)$$

with n even. Thus we indicate in this subsection by x_j the zeros of this polynomial, which satisfy, in the notation of Sec. 1, the equations

$$\xi_j = x_j + x_j^{-1}, \quad j = 1,2,...,n, \qquad (4.3.2)$$

$$\xi_j^{(2)} = \tfrac{1}{3}[2(n-2) - x_j^2 + x_j^{-2}]. \qquad (4.3.3)$$

The first of these equations is taken from Ref. 12: the second can be easily derived from the results of Ref. 12, for instance by the technique used in Ref. 13.

These formulas may be used, in conjunction with those of Sec. 1 [see, in particular, (1.10) and (1.17)], to obtain more explicit and compact expressions of the matrices $\mathbf{Z}$ and $\mathbf{Z}^2$—hence of all the matrices appearing in Sec. 3, whose results are, of course, all applicable.

Note that (3.18b), together with

$$H_n(\mathbf{X}) = -2nH_{n-2}(\mathbf{X}), \qquad (4.3.4)$$

[implied by (4.3.1)] and (3.18b), yields

$$(2\mathbf{X}-\mathbf{Z})\mathbf{v}^{(H)(n)} = -2n\,\mathbf{v}^{(H)(n-1)}, \qquad (4.3.5)$$

and this, together with (3.17), gives

$$\mathbf{X}\mathbf{v}^{(H)(n)} = -\mathbf{v}^{(H)(n-1)}. \qquad (4.3.6)$$

There is, however, no neat way to define a proper "raising" operator, namely a matrix having the property (3.18a) and, in addition, annihilating $\mathbf{v}^{(n)}$.

4.4. Matrices constructed with the zeros of Laguerre polynomials

In this subsection we take for the polynomial (1.1) the choice

$$p_n(x) = (-)^n[\Gamma(n+\alpha+1)/n!]^{-1/2}L_n^\alpha(x). \quad (4.4.1)$$

The normalization constant is introduced to make the notation consistent with that of Sec. 2, with in addition

$$a=0, \quad b=\infty, \quad w(x)=x^\alpha\exp(-x),$$
$$k_n = \left[\Gamma(\alpha+1)\binom{n+\alpha}{n}\right]^{-1/2}(n!)^{-1}. \qquad (4.4.2)$$

Thus, throughout this subsection, the x_j's are the n zeros of the (generalized) Laguerre polynomial[10] of order n:

$$L_n^\alpha(x_j)=0, \quad j=1,2,...,n. \qquad (4.4.3)$$

These numbers depend, of course, on n and α, but this is not explicitly indicated here for notational simplicity.

This choice yields, in the notation of Secs. 1 and 2,[3]

$$\xi_j = \tfrac{1}{2}\,[1-(1+\alpha)/x_j], \qquad (4.4.4)$$

$$\xi_j^{(2)} = -\tfrac{1}{12}\,[1-2(2n+1+\alpha)/x_j+(\alpha+1)(\alpha+5)/x_j^2], \qquad (4.4.5)$$

$$c_j = x_j^{1/2}, \qquad (4.4.6)$$

$$u_m^{(j)} = (-)^{n-m}\left(\frac{x_j\Gamma(n+\alpha)(m-1)!}{(n+\alpha)\Gamma(m+\alpha)n!}\right)^{1/2}\frac{L_{m-1}^\alpha(x_j)}{L_{n-1}^\alpha(x_j)}. \qquad (4.4.7)$$

These equations, in particular (4.4.4) and (4.4.5), can be combined with the results of Sec. 3. The neater results obtain in connection with those of Propositions 3.3. and 3.6. Their relation to the results of Sec. 4 of Ref. 3 is given by the formula

$$\mathbf{N}^{(L)} = (n-1)\mathbf{I}-2\mathbf{X}\mathbf{B}\mathbf{X}^{-1}, \qquad (4.4.8)$$

where $N^{(L)}$ is defined by (3.20) and $\mathbf{B}$ by Eq. (4.4) of Ref. 3. The results of Ref. 7 are, moreover, reproduced, with the following notational correspondence:

$$\mathbf{A} = \tfrac{1}{2}\mathbf{C}^{-1}[(n-1)\mathbf{I}-\mathbf{N}^{(L)}]\mathbf{C}, \qquad (4.4.9)$$

$$\mathbf{A}^{(\pm)} = \mathbf{C}^{-1}\mathbf{L}^{(\pm)}\mathbf{C}, \qquad (4.4.10)$$

$$\mathbf{v}^{(m)} = (-)^{n+1}[\Gamma(\alpha+m)/(m-1)!]^{-1/2}\mathbf{C}^{-1}\mathbf{v}^{(L)(m)}, \qquad (4.4.11)$$

with [see (4.4.6)]

$$\mathbf{C} = \mathbf{X}^{1/2}. \qquad (4.4.12)$$

The matrices and vectors in the lhs of (4.4.9), (4.4.10), and (4.4.11) are defined in Ref. 7, while those in the rhs are defined in the present paper, see in particular (3.20), (3.25), and (3.21) [the latter, of course, with (1.4) and (4.4.1)]. Finally, the results of Sec. 2 are also applicable, with the orthonormal set defined according to (4.4.1) and (4.4.2) and the quantities $u_m^{(j)}$ and c_j defined by (4.4.6) and (4.4.7); the appropriate definition of the operators $\mathscr{A}$ and $\mathscr{A}^{(\pm)}$ of Sec. 2, such that the matrices $\mathbf{A}$ and $\mathbf{A}^{(\pm)}$ of Sec. 2 coincide with those introduced here, (4.4.9) and (4.4.10), then read

$$\mathscr{A} = \tfrac{1}{2}[n-1-(x-1-\alpha)\,d/dx+x\,d^2/dx^2], \qquad (4.4.13)$$

$$\mathscr{A}^{(-)} = (1+\alpha+x\,d/dx)\,d/dx, \qquad (4.4.14a)$$

$$\mathscr{A}^{(+)} = -2x\,d/dx-(1+\alpha)(1-d/dx)+x(1+d^2/dx^2), \qquad (4.4.14b)$$

namely, they are just (up to a sign; see below) the translation into differential operators (according to the simple rule $\mathbf{X}\to x$, $\mathbf{Z}\to d/dx$) of the matrices

$$\tilde{\mathbf{A}} = \mathbf{C}\mathbf{A}\mathbf{C}^{-1} = \tfrac{1}{2}[(n-1)\mathbf{I}-\mathbf{N}^{(L)}], \qquad (4.4.15)$$

$$\tilde{\mathbf{A}}^{(\pm)} = -\mathbf{C}\mathbf{A}^{(\pm)}\mathbf{C}^{-1} = -\mathbf{L}^{(\pm)}, \qquad (4.4.16)$$

as implied by Proposition 2.1. The corresponding values of the quantities $\alpha_m^{(\pm)}$ and a_m are

$$\alpha_m^{(-)} = [(m-1)(m-1+\alpha)]^{1/2},$$
$$\alpha_m^{(+)} = [m(m+\alpha)]^{1/2}, \qquad (4.4.17)$$

$$a_m = \tfrac{1}{2}(n-m), \qquad (4.4.18)$$

consistently with the differential formulas

$$\mathscr{A}^{(\pm)}p_{p-1}(x) = \alpha_p^{(\pm)}p_{p-1\pm1}(x), \qquad (4.4.19)$$

$$\mathscr{A}p_{p-1}(x) = a_p p_{p-1}(x), \qquad (4.4.20)$$

where, of course,

$$p_p(x) = (-)^p[\Gamma(p+1+\alpha)/p!]^{-1/2}L_p^\alpha(x), \quad (4.4.21)$$

and with the corresponding vector formulas,[7]

$$\mathbf{A}^{(-)}\mathbf{v}^{(m)} = \alpha_m^{(-)}\mathbf{v}^{(m-1)}, \quad m=1,2,...,n, \qquad (4.4.22a)$$

$$\mathbf{A}^{(+)}\mathbf{v}^{(m)} = [\alpha_m^{(+)}-\delta_{mn}\alpha_n^{(+)}]\mathbf{v}^{(m+1)}, m=1,2,...,n, \qquad (4.4.22b)$$

$$\mathbf{A}\mathbf{v}^{(m)} = a_m\mathbf{v}^{(m)}. \qquad (4.4.23)$$

Here the vectors $\mathbf{v}^{(m)}$ are defined by (4.4.11), and it is easily seen that this definition is consistent (up to a sign factor) with that of the normalized vectors of Sec. 2; indeed

$$\mathbf{v}^{(m)} = (-)^{n-m}\tilde{\mathbf{u}}^{(m)}, \qquad (4.4.24)$$

[see (4.4.11), (4.4.7), and (2.23)]. Note the consistency of the sign factor in (4.4.24) with the minus sign in (4.4.16).

Let us emphasize again that here, besides reproducing the results of Refs. 3 and 7, we have clarified their relation to the general theory of orthogonal polynomials by displaying the connection with the treatment of Sec. 2.

As in the case of Hermite polynomials, see Sec. (4.2), it is of course possible to combine the special choice of the set x_j considered in this subsection with other results of Sec. 3 besides Propositions 3.3 and 3.6; but this is left as an exercise for the diligent reader.

4.5. Matrices constructed with the zeros of Jacobi polynomials

In this subsection we limit our presentation to providing, without commentary, the formulas needed to relate the treatment given in this paper with the results of Ref. 3 involving the zeros of Jacobi polynomials. Thus we set

$$p_n(x)=\left(\frac{2^{\alpha+\beta+1}\Gamma(n+\alpha+1)\Gamma(n+\beta+1)}{(2n+\alpha+\beta+1)n!\Gamma(n+\alpha+\beta+1)}\right)^{-1/2}\times P_n^{(\alpha,\beta)}(x), \quad (4.5.1)$$

implying of course that in this subsection the numbers x_j are the n zeros of the Jacobi polynomial of order n,

$$P_n^{(\alpha,\beta)}(x_j)=0, \quad j=1,2,...,n. \quad (4.5.2)$$

The results of Sec. 2 are then applicable for the orthonormal set of polynomials

$$p_p(x)=\left(\frac{2^{\alpha+\beta+1}\Gamma(p+\alpha+1)\Gamma(p+\beta+1)}{(2p+\alpha+\beta+1)p!\Gamma(p+1+\alpha+\beta)}\right)^{-1/2}\times P_p^{(\alpha,\beta)}(x), \quad (4.5.3)$$

with

$$a=-1, \quad b=+1, \quad w(x)=(1-x)^\alpha(1+x)^\beta,$$

$$k_n=[2^{2n+\alpha+\beta+1}(2n+\alpha+\beta+1)n!\Gamma(n+1+\alpha)\times\Gamma(n+1+\beta)\Gamma(n+1+\alpha+\beta)]^{-1/2}\times\Gamma(2n+2+\alpha+\beta), \quad (4.5.4)$$

$$c_j=[(1-x_j^2)n/(2n+1+\alpha+\beta)]^{1/2}, \quad (4.5.5)$$

$$u_m^{(j)}=\tfrac{1}{2}(2n+\alpha+\beta)\times\{[(2m+\alpha+\beta-1)(m-1)!\times\Gamma(m+\alpha+\beta)\Gamma(n+\alpha)\Gamma(n+\beta)]\times[n(n+\alpha)(n+\beta)n!\Gamma(n+\alpha+\beta+1)\times\Gamma(m+\alpha)\Gamma(m+\beta)]^{-1}\}^{1/2}\times(1-x_j^2)^{1/2}P_{m-1}^{(\alpha,\beta)}(x_j)/P_{n-1}^{(\alpha,\beta)}(x_j). \quad (4.5.6)$$

There hold, moreover, the relations[3]

$$\xi_j=\tfrac{1}{2}[\alpha-\beta+(\alpha+\beta+2)x_j]/(1-x_j^2), \quad (4.5.7)$$

$$\xi_j^{(2)}=\tfrac{1}{12}\{4(n-1)(\alpha+\beta+n+2)-(\alpha-\beta)^2-2(\alpha-\beta)(\alpha+\beta+6)x_j-[4n(\alpha+\beta+n+1)+(\alpha+\beta+2)(\alpha+\beta+6)]x_j^2\}/(1-x_j^2)^2, \quad (4.5.8)$$

implying (after a tedious computation)

$$\Gamma=\tfrac{1}{2}\mathbf{C}^{-2}[(n-1)(n+\alpha+\beta)\mathbf{I}-\mathbf{N}^{(J)}]\mathbf{C}^2, \quad (4.5.9)$$

with **I** the unit matrix, $\mathbf{N}^{(J)}$ defined by (3.30), **C** defined by (2.39) and (4.5.5), and with the matrix Γ defined by

$$\Gamma_{jk}=\delta_{jk}\sum_{l=1}^{n}{}'(1-x_l^2)/(x_j-x_l)^2-(1-\delta_{jk})(1-x_k^2)/(x_j-x_k)^2. \quad (4.5.10)$$

Thus Γ coincides with the matrix **C** defined by Eq. (5.4) of Ref. 3, and Eq. (4.5.9) provides the connection with the results of Ref. 3.

5. OUTLOOK

Several directions of further research are naturally suggested by the results reported in this paper.

In the first place the limit of these results as $n\to\infty$ should be studied. In this manner it should be possible to obtain results on the spectrum of infinite matrices such as those discussed in Ref. 3 and on the properties of integral singular operators such as those considered in Ref. 14. Particularly interesting should be the relationships that shall thus arise between differential operators, infinite matrices and singular integral operators.

Secondly, the results of this paper suggest investigating the use of the matrix **Z** as an (approximate) representation of the differential operator in the context of numerical analysis and of the problems of interpolation, of mechanical quadrature, and of the numerical solution of (differential and integrodifferential) eigenvalue problems. In the latter context the extension to more than one variable is also appealing.

The question of confluence should also be considered, namely the limiting form taken by the results of this paper (see in particular Secs. 1 and 2) if two, or more, of the *a priori* arbitrary (but different) numbers x_j coalesce.

Let us finally note that, in this paper, nothing has been said on the "inverse" problems in which a matrix, having a certain structure that defines it in terms of a set of numbers, is required to have a given spectrum, and this requirement is supposed to determine the (*a priori* unknown) set of numbers. We know, of course, that in some cases this problem has either no solution or too many solutions; for instance, the requirement that the matrix **N**, of order n, defined by (I.3), have a given spectrum, has generally no solution, unless the spectrum coincides with the first n nonnegative integers, in which case no restriction at all is implied on the numbers x_j. On the other hand, it has been conjectured[1-3] that the requirement that the matrix **A**, of order n, defined by (I.1), have the first n nonnegative integers as eigenvalues, implies that the numbers x_j coincide, up to a common additive constant, with the n zeros of the Hermite polynomial of order n; and many analogous conjectures[3] can be plausibly formulated [for instance, in terms of the matrices defined by (4.2.14) or (4.2.15)]. All these conjectures stand; and, while the hope that the more general approach developed in this paper provides a handle to prove or disprove them appears reasonable, so far I cannot report any substantive progress.

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APPENDIX A

The main formula to prove is (2.9). For $j\neq k$ the proof is easy: the definition (2.7) implies

$$p_{n-1}^{(j)}(x)p_{n-1}^{(k)}(x)=q_{n-2}(x)p_n(x), \quad (A1)$$

q_{n-2} being a polynomial of degree $n-2$ and being, therefore, orthogonal to $p_n(x)$ [see (2.1)]. For $j=k$, it is convenient to assume that (2.9) holds, since this can always be enforced by appropriate choice of the normalization constants c_j in (2.7); the actual evaluation of c_j, namely, the proof of (2.8), is postponed. The formulas (2.10), (2.11), and (2.12) are obvious. It is then convenient to go over to (2.17) and (2.18), while *define* $u_m^{(j)}$, and to notice that these formulas, together with (2.1) and (2.9), imply (2.19) and (2.20).

Then (2.13a) is proved, using (2.17)–(2.20); (2.13b) follows, using 02.2); next follows (2.14), in an obvious way, (2.15) from (2.13a) and (2.11b), and (2.16) also trivially; and then (2.21) follows, from a comparison of (2.15) with (2.17). Now inserting (2.21) in (2.19) and using the formula

$$\sum_{m=1}^{n} p_{m-1}(x_j)p_{m-1}(x_k) = \delta_{jk}(k_{n-1}/k_n)p_n'(x_j)p_{n-1}(x_j), \tag{A2}$$

which is a special case of (2.2) and (2.3), we finally obtain (2.8). The proof of the remaining equations is plain: (2.27) and (2.28) follow from (2.26), using (2.17)–(2.20) and (2.23) and in a similar manner (2.30) and (2.31) follow from (2.29); (2.33) follows from (2.27), and similarly (2.34) from (2.30).

APPENDIX B

The proof of (4.1.6a) is trivial :

$$\sum_{l=1}^{n}{}' \{1-\exp[2\pi i(l-j)/n]\}^{-1} = \sum_{l=1}^{n-1} [1-\exp(2\pi i l/n)]^{-1}, \tag{B1}$$

$$\sum_{l=1}^{n-1} [1-\exp(2\pi i l/n)]^{-1} = n-1+\sum_{l=1}^{n-1} [1-\exp(2\pi i l/n)]^{-1}\exp(2\pi i l/n) \tag{B2a}$$

$$= n-1-\sum_{l=1}^{n-1} [1-\exp(2\pi i l/n)]^{-1}. \tag{B2b}$$

The step (B1) is obtained by replacing the summation index l with $l'=l-j$, and using the cyclic property. The step (B2a) is obtained by multiplying the summand by $[1-\exp(2\pi i l/n)]+\exp(2\pi i l/n)$; (B2b) is obtained by replacing the summation index l by $n-l$, and it clearly yields (4.1.6a) . Q.E.D.

The proof of (4.1.6b) is also plain:

$$\sum_{l=1}^{n}{}' \{1-\exp[2\pi i(l-j)/n]\}^{-2} = \sum_{l=1}^{n-1} [1-\exp(2\pi i l/n)]^{-2}, \tag{B3}$$

$$\sum_{l=1}^{n-1} [1-\exp(2\pi i l/n)]^{-2} = \tfrac{1}{2}(n-1)+\sum_{l=1}^{n-1} [1-\exp(2\pi i l/n)]^{-2} \times\exp(2\pi i l/n) \tag{B4a}$$

$$= \tfrac{1}{2}(n-1)-\tfrac{1}{4}\sum_{l=1}^{n-1} [\sin(\pi l/n)]^{-2} \tag{B4b}$$

$$= \tfrac{1}{2}(n-1)-\tfrac{1}{12}(n^2-1). \tag{B4c}$$

The steps (B3) and (B4a) are analogous to (B1) and (B2a); (B4b) is plain; (B4c) is obtained from Eqs. (14) and (8) of Ref. 11, and it yields (4.1.6b) . Q.E.D.

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Explicit evaluation of the representation functions of IU(n)

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All representation functions of IU(n) have been found in explicitly closed form. They are obtained through the contraction of U($n+1$) or U(n,1). These expressions are closely connected with the generalized beta functions of Gel'fand and Graev.

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I. INTRODUCTION

In a previous paper,[1] we have obtained an explicit expression for the representation functions of ISO(n). In this paper we show how the representation functions of IU(n) can be explicitly obtained.

The method used in this paper, however, is quite different from that of Ref. 1. Whereas in the case of ISO(n), we obtained the representation functions through the method of induced representations as given by Wolf[2] in the form of an integral, we find that this method is not easy to use in the case of IU(n), even though Wolf[3] has in fact given an integral expression for IU(n). In Ref. 1, we mentioned that the representation functions of ISO(n) can also be obtained from the contraction of the representation functions of SO($n+1$) or SO(n, 1), through Wigner's method.[4,5] We showed there explictly how the d-functions of ISO(2) and ISO(3) can be obtained from the d-functions of SO(3) and SO(4) respectively through the process of contraction. In a future publication we shall show that this contraction process, when applied to ISO(n), will lead to a new result different from that in Ref. 1, in that the representation functions of ISO(n) are expressible as sums over a confluent hypergeometric function ${}_1F_1$ with argument $2i\gamma\xi$. This contraction process is also valid when applied to IU(n). In other words, we are saying that IU(n) can be considered as derivable from U($n+1$) or U(n, 1) through the process of contraction. In the case of IU(n), we find that this method of contraction is much easier to use than the method of induced representation through integration. Thus we intend to show in this paper how an explicit expression for the representation functions of IU(n) can be obtained from contracting the representation functions of U($n+1$) or U(n, 1).

There are at least two different ways of writing the representation functions of U(n): one by means of the Weyl coefficients,[6] and the other by the generalized beta functions of Gel'fand and Graev.[7] The first one, however, cannot be easily extended to U(n, 1), whereas the second one can be extended to U(n, 1), as done by Klimyk and Gavrilik.[8] If the contraction process is to give meaningful results, the representation functions chosen to be contracted must be applicable to both U($n+1$) and U(n, 1). Thus we must use the representation functions given by Gel'fand and Graev. The final expression we have obtained for the representation functions of IU(n) is in terms of powers of $\kappa\xi$, summed over n variables. Here κ is the same continuous variable used by Chakrabarti,[9] and $|\kappa|^2$ is the eigenvalue of the second order Casimir invariant of IU(n), i.e.,

$$\Delta_{(2)} = \sum_{i=1}^{n} I_i^{n+1} I_{n+1}^{i} = |\kappa|^2. \tag{1.1}$$

ξ is the same variable used by Wolf.[3] It represents translation in the n direction. This expression is convergent for all values of κ and ξ, and can also be expressed as a finite sum over a generalized hypergeometric function ${}_{3(n-1)}F_{3n-2}$ for IU(n). It is interesting to note that this expression is quite different from that of ISO(n), $n>2$, where, as we have shown in Ref. 1, the representation functions are expressible as a summation over Bessel functions. The only exception, of course, is in the case of IU(1) which has the same form as that of ISO(2), i.e., as an ordinary Bessel function.

In Sec. II, we discuss briefly the representation theory of IU(n), and its relation to U($n+1$) and U(n, 1). In Sec. III, we calculate explicitly the representation function of IU(1), which is somewhat special, because it has the same form as ISO(2). In Sec. IV, we calculate explicitly the representation function of IU(2). In Sec. V we obtain the general representation functions for all IU(n).

II. SUMMARY OF THE THEORY OF REPRESENTATIONS OF IU(N), U($N+1$), AND U(N,1)

The main results connecting the representations of IU(n), U($n+1$), and U(n, 1) are contained in a paper of ours.[10] Here we shall mention only those formulas and notations that are necessary for the understanding of subsequent sections.

For IU($n-1$) we denote the basis state by

$$\left| \begin{matrix} & m_{2,n} & \cdots m_{n-1,n} \\ m_{1,n-1} & m_{2,n-1} & \cdots m_{n-1,n-1} \\ & & \cdots \\ m_{1,1} & & \end{matrix} \right\rangle . \tag{2.1}$$

For the continuous variable we use κ according to

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Chakrabarti.[9] [See Eq. (1.1).] For U(n) we denote the basis state by

$$\left| \begin{matrix} m_{1,n} m_{2,n} \cdots m_{n,n} \\ m_{1,n-1} \quad \cdots m_{n-1,n-1} \\ \cdots \\ m_{1,1} \end{matrix} \right\rangle . \tag{2.2}$$

For U($n-1,1$) we denote the basis state also by (2.2) with the understanding that, for the principal continuous series,

$$\begin{aligned} m_{1,n} &= -(n-1)/2 + z, \\ m_{n,n} &= (n-1)/2 + z^*. \end{aligned} \tag{2.3}$$

The contraction process then goes as follows:

For ISO(n), we showed in Ref. 1 that

$$m_{1,n+1}\theta = \gamma\xi, \text{ and } m_{1,n+1} \to \infty. \tag{2.4}$$

A similar result is found for IU(n) (see Wolf[3]), i.e.,

$$\epsilon\theta = \kappa\xi \text{ and } \epsilon \to \infty, \tag{2.5}$$

where $\epsilon = \mathrm{Im} z$. This is equivalent to

$$m_{1,n} \to i\infty$$

and (2.6)

$$m_{n,n} \to -i\infty.$$

Then the only formula one has to use in the contraction process is the one given by Talman[11]:

$$\lim_{n\to\infty}[(n+p)!\,(n+q)!] = \lim_{n\to\infty}(n)^{p-q}. \tag{2.7}$$

III. EXPLICIT EVALUATION OF THE REPRESENTATION FUNCTION OF IU(1)

Before going to the particular cases, we would like to derive the d-functions of U(n) according to the method of Gel'fand and Graev.

Any element g of U(n) can be decomposed uniquely as

$$g = h a(\phi) b(\theta) \tilde{h}, \tag{3.1}$$

where $a(\phi)$ and $b(\theta)$ are the matrices

$$a(\phi) = \begin{pmatrix} 1 & 0 & & \\ 0 & 1 & & \\ & & \ddots & \\ & & & e^{-i\phi} \end{pmatrix}; \quad b(\theta) = \begin{pmatrix} 1 & 0 & & \\ 0 & 1 & & \\ & & \cos\theta & -\sin\theta \\ & & \sin\theta & \cos\theta \end{pmatrix}, \tag{3.2}$$

h is the most general element of the subgroup U($n-1$), and $\tilde{h}$ is a special element of U($n-1$). But $b(\theta)$ can be further decomposed as follows:

$$b(\theta) = \begin{pmatrix} 1 & 0 & & \\ 0 & 1 & & \\ & & 1 & 0 \\ & & \tan\theta & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & & \\ 0 & 1 & & \\ & & \cos\theta & 0 \\ & & 0 & (\cos\theta)^{-1} \end{pmatrix} \begin{pmatrix} 1 & 0 & & \\ 0 & 1 & & \\ & & 1 & -\tan\theta \\ & & 0 & 1 \end{pmatrix} = b(I + te_{n,n-1}) b_0(\theta) b(I - te_{n-1,n}), \tag{3.3}$$

where $t = \tan\theta$.

The d-functions of $b(I + te_{n,n-1})$ and $b(I + te_{n,n-1})$ have been given by Gel'fand and Graev.[7] They can also be expressed in terms of the isoscalar factors of U(n) and U($n-1$) for the totally symmetric representations; as shown by Louck and Biedenharn.[11]

Thus for IU(1), we have

$$\begin{aligned} & d^{m_{12},m_{22}}_{m'_{11}m_{11}}(\theta) \to {}^I d^{\kappa}_{m'_{11}m_{11}}(\xi), \\ & \epsilon\theta = \kappa\xi, \\ & \epsilon \to \infty. \end{aligned} \tag{3.4}$$

Now we write the d-function of U(2) according to (3.3), i.e.,

$$d^{m_{12}m_{22}}_{m'_{11}m_{11}}(\theta) = \sum_{m''_{11}} d^{m_{12}m_{22}}_{m'_{11}m''_{11}}(I + te_{21}) \times d^{m_{12}m_{22}}_{m''_{11}m''_{11}}(b_0(\theta)) d^{m_{12}m_{22}}_{m''_{11}m_{11}}(I - te_{12}). \tag{3.5}$$

According to Louck and Biedenharn.

$$d^{m_{12}m_{22}}_{m'_{11}m_{11}}(I + te_{12}) = \left[\frac{\mathfrak{M}(m_{12}, m_{22})}{\mathfrak{M}(m_{11})}\right]^{1/2} \times \frac{S_{21}(m_{12}, m_{22}; m_{11}) S_{22}(m_{12}, m_{22}; m_{12}, m_{22})}{S_{21}(m'_{11}, 0; m_{11}) S_{22}(m_{12}, m_{22}; m'_{11}, 0)} \times \frac{S_{11}(m'_{11}; m'_{11})}{S_{11}(m'_{11}; m_{11})}\, t^{m'_{11} - m_{11}}, \tag{3.6}$$

where

$$\mathfrak{M} = \prod_{i=1}^{n} (m_{in} + n - i) \Big/ \prod_{i<j}^{n} (m_{in} - m_{jn} + j - i), \tag{3.7}$$

$$S_{nm}(h_1 \ldots h_n; q_1 \ldots q_m) = \left[\frac{\prod_{k=1}^{m}\prod_{s=1}^{k} (h_s - q_k + k - s)!}{\prod_{k=1}^{n-1}\prod_{s=k+1}^{n} (q_k - h_s + s - k - 1)!}\right]^{1/2}, \tag{3.8}$$

$$d^{m_{12}m_{22}}_{m''_{11}m''_{11}}(b_0(\theta)) = (\cos\theta)^{m''_{11}} (\cos\theta)^{-m_{12} - m_{22} + m''_{11}}, \tag{3.9}$$

$$d^{m_{12}m_{22}}_{m_{11}m''_{11}}(I + te_{21}) = d^{m_{12}m_{22}}_{m''_{11}m_{11}}(I + te_{12}). \tag{3.10}$$

If we write out (3.5) explicitly, we obtain the d-function of U(2) as

$$d^{m_{12}m_{22}}_{m'_{11}m_{11}}(\theta)=\sum_{m''_{11}}\left[\frac{(m_{12}-m'_{11})!(m_{12}-m_{11})!}{(m'_{11}-m_{22})!(m_{11}-m_{22})!}\right]^{1/2} \times\frac{(m''_{11}-m_{22})!(-1)^{m''_{11}-m_{11}}}{(m_{12}-m''_{11})!(m''_{11}-m'_{11})!(m''_{11}-m_{11})!} \times(\cos\theta)^{m_{11}+m'_{11}-m_{12}-m_{22}}(\sin\theta)^{2m''_{11}-m_{11}-m'_{11}}. \tag{3.11}$$

This formula with θ replaced by $\theta/2$ is in agreement with the d-function of U(2) as given by Rose,[12] Eq. (4.14).

Applying the contraction process and Eq. (2.7) to Eq. (3.5), we obtain the d-function of IU(1):

$$^I d^{\kappa}_{m'_{11}m_{11}}(\xi)=\sum_{m''_{11}}\frac{1}{(m''_{11}-m_{11})!(m''_{11}-m'_{11})!} \times(-1)^{m''_{11}-m_{11}}(\kappa\xi)^{2m''_{11}-m_{11}-m'_{11}}. \tag{3.12}$$

By redefining $m=m''_{11}-m'_{11}$ we find

$$\begin{aligned}^I d^{\kappa}_{m'_{11}m_{11}}(\xi)&=\sum_{m}\frac{1}{m!(m+m'_{11}-m_{11})!}\times(-1)^{m+m'_{11}-m_{11}}(\kappa\xi)^{2m+m'_{11}-m_{11}}\\&=(-1)^{m'_{11}-m_{11}}J_{m'_{11}-m_{11}}(2\kappa\xi)\\&=J_{m_{11}-m'_{11}}(2\kappa\xi).\end{aligned} \tag{3.13}$$

This result, of course, can also be obtained by contracting the Jacobi polynomial, as we pointed out in Ref. 1, Eq. (2.7). Thus if we write the d-function of U(2) in terms of the Jacobi polynomial:

$$d^j_{m'm}(\beta)=(-1)^{m-m'}\left[\frac{(j+m')!(j-m')}{(j+m)!(j-m)}\right]^{1/2}(\cos\beta/2)^{m'+m} \times(\sin\beta/2)^{m'-m}P^{(m'-m,m'+m)}_{j-m'}(\cos\beta) \tag{3.14}$$

we can use the contraction process [Ref. 13, Eq. (41), p. 173]

$$\lim_{n\to\infty} n^{-\alpha}P_n^{(\alpha,\beta)}(\cos(z/n))=(z/2)^{-\alpha}J_\alpha(z) \tag{3.15}$$

and obtain

$$^I d^{\kappa}_{m'_{11}m_{11}}(\xi)=J_{m_{11}-m'_{11}}(2\kappa\xi). \tag{3.16}$$

Note that in Eq. (3.14) we have added the phase $(-1)^{m-m'}$ to the d-function of U(2) as given by Edmonds, Eq. (4.123).[14] This is because the d-function of Edmonds differs from that of Rose by the phase factor $(-1)^{m-m'}$. Also it is obvious that β in Eq. (3.14) is equal to 2θ in Eq. (3.11). This explains the factor $2\kappa\xi$ as the argument of the Bessel function in Eq. (3.16).

The result of IU(1), of course, reminds one of the representation function of ISO(2), which is of the same form. However, one must not conclude that the representation function of IU(n) will be similar to those of ISO(n), as we shall show in subsequent sections. In a sense, therefore, IU(1) is a special case.

IV. EXPLICIT EVALUATION OF THE REPRESENTATION FUNCTION OF IU(2)

For the case of IU(2), we start by writing down the d-function of U(3) according to Eq. (3.3).

$$d^{m_{13}m_{23}m_{33}}_{\substack{m_{12}m_{22}m'_{12}m'_{22}\\ m_{11}\quad m_{11}}}(\theta) =\sum_{m''_{12}m''_{22}} d^{m_{13}m_{23}m_{33}}_{\substack{m_{12}m_{22}m''_{12}m''_{22}\\ m_{11}\quad m_{11}}}(I+\tan\theta e_{32})(\cos\theta)^{m''_{12}+m''_{22}-m_{11}} \times(\cos\theta)^{m''_{12}+m''_{22}-m_{13}-m_{23}-m_{33}}d^{m_{13}m_{23}m_{33}}_{\substack{m''_{12}m''_{22}m'_{12}m'_{22}\\ m_{11}\quad m_{11}}}(I-\tan\theta e_{23}). \tag{4.1}$$

The d-functions of $(I+te_{32})$ and $(I-te_{23})$ have, in fact, been explicitly given by Gel'fand and Graev.[7] Note that their basis is modified by a factor $\lambda(m)$ given in Eq. (2.2) of their paper. Thus Eq. (4.1) can be written down explicitly. The important point we wish to make is that in the contraction process, the terms containing infinity all cancel out. To demonstrate this, let us pick out from Eq. (4.1) only those terms which approach infinity, i.e., terms containing m_{13} and m_{33}. Then we have

$$\left[\frac{(m_{13}-m_{12})!(m_{13}-m_{22}+1)!(m''_{12}-m_{33}+1)!(m''_{22}-m_{33})!}{(m_{13}-m''_{12})!(m_{13}-m''_{22}+1)!(m_{12}-m_{33}+1)!(m_{22}-m_{33})!}\right]^{1/2} \times\left(\frac{\kappa\xi}{\epsilon}\right)^{m''_{12}+m''_{22}-m_{22}-m_{12}} \tag{4.2}$$

and a similar term with m_{12} and m_{22} replaced by m'_{12} and m'_{22} respectively. It is clear that by applying the limiting process of (2.5)–(2.7) to (4.2), we find that (4.2) is reduced to

$$(\kappa\xi)^{m''_{12}+m''_{12}-m_{12}-m_{22}}. \tag{4.3}$$

Thus all terms containing infinity drop out.

Thus we obtain the representation function of IU(2) explicitly as follows:

$$^I d^{\kappa m_{23}}_{\substack{m_{12}m_{22}m'_{12}m'_{22}\\ m_{11}\quad m_{11}}}(\xi)=\left[\frac{(m_{23}-m_{22})!(m_{11}-m_{22})!(m_{23}-m'_{22})!(m_{11}-m'_{22})!}{(m_{12}-m_{23})!(m_{12}-m_{11})!(m'_{12}-m_{23})!(m'_{12}-m_{11})!}\right]^{1/2} \times[(m_{12}-m_{22}+1)(m'_{12}-m'_{22}+1)]^{1/2} \times\sum_{m''_{12}m''_{22}}\frac{(m''_{12}-m_{23})!(m''_{12}-m_{11})!(m_{12}-m''_{22})!(m'_{12}-m''_{22})!(m''_{12}-m''_{22}+1)}{(m_{23}-m''_{22})!(m_{11}-m''_{22})!(m''_{12}-m_{22}+1)!(m''_{12}-m'_{22}+1)!(m''_{12}-m_{12})!} \times\frac{1}{(m''_{12}-m'_{12})!(m''_{22}-m_{22})!(m''_{22}-m'_{22})!}(\kappa\xi)^{2m''_{12}-m_{12}-m_{22}-m'_{12}-m'_{22}+2m''_{22}}. \tag{4.4}$$

Equation (4.4) can be rewritten in different forms as sums over a generalized hypergeometric series. From the expression in (4.4) it is easy to see that the summation over m''_{12} is an infinite sum, while the summation over m''_{22} is finite. It is easy to check that the expression in (4.4) is convergent for all values of κ and ξ. We shall see in the next section that the two properties mentioned above are applicable to all the representation functions of IU(n), $n>1$. The two properties are: (1) The representation functions of IU(n) are convergent for all values of κ and ξ. (2) They can be expressed as sums over generalized hypergeometric functions.

V. REPRESENTATION FUNCTIONS OF IU(n)

The process we have used for IU(1) and IU(2) can be generalized to IU(n). The d-function of U($n+1$) is written as

$$d^{[m]_{n+1}}_{\substack{[m]_n[m']_n\\ [m]_{n-1}[m]_{n-1}}}(\theta)=\sum_{[m'']_n} d^{[m]_{n+1}}_{\substack{[m]_n[m'']_n\\ [m]_{n-1}[m]_{n-1}}}(I+te_{n+1,n})(\cos\theta)^{W''_n-W''_{n+1}} \times d^{[m]_{n+1}}_{\substack{[m'']_n[m']_n\\ [m]_{n-1}[m]_{n-1}}}(I-te_{n,n+1}), \qquad (5.1)$$

where

$$W_n=\sum_{i=1}^{n} m_{in}-\sum_{j=1}^{n-1} m_{jn-1}.$$

For the d-functions appearing on the right-hand side of Eq. (5.1), we can use the expression obtained explicitly by Louck and Biedenharn.[11]

$$d^{[m]_n}_{\substack{[m]_{n-1}[m]_{n-1},\\ [m]_{n-2}[m]_{n-2}}}(I+te_{n,n-1})=d^{[m]_n}_{\substack{[m]_{n-1}[m]_{n-1},\\ [m]_{n-2}[m]_{n-2}}}(I+te_{n-1,n})$$
$$=\left[\frac{\mathfrak{M}([m]_n)}{b!\,b'!\,\mathfrak{M}([m]_{n-1})}\right]^{1/2}\left\langle\begin{matrix}[m]_n\\ [m]_{n-1}\end{matrix}\middle|\begin{matrix}b,\dot{0}\\ 0\end{matrix}\middle|\begin{matrix}[m']_{n-1}0\\ [m]_{n-1}\end{matrix}\right\rangle \times\left\langle\begin{matrix}[m']_{n-1}\\ [m]_{n-2}\end{matrix}\middle|\begin{matrix}b',\dot{0}\\ 0\end{matrix}\middle|\begin{matrix}[m]_{n-1}\\ [m]_{n-2}\end{matrix}\right\rangle t^{b'}, \qquad (5.2)$$

where the measure $\mathfrak{M}$ is given in Eq. (3.7), and

$$\left\langle\begin{matrix}[m]_n\\ [m]_{n-1}\end{matrix}\middle|\begin{matrix}b,\dot{0}\\ 0\end{matrix}\middle|\begin{matrix}[m']_n\\ [m]_{n-1}\end{matrix}\right\rangle=(b!)^{\frac{1}{2}} \times\frac{S_{nn-1}(m_{1n}\cdots m_{n,n};m_{1n-1}\cdots m_{n-1,n-1})}{S_{nn-1}(m'_{1n}\cdots m'_{n,n};m_{1n-1}\cdots m_{n-1,n-1})} \times\frac{S_{nn}(m_{1n}\cdots m_{nn};m_{1n}\cdots m_{nn})}{S_{nn}(m_{1n}\cdots m_{nn};m'_{1n}\cdots m'_{nn})} \qquad (5.3)$$

$$b=\sum_{i=1}^{n} m_{in}-\sum_{i=1}^{n-1} m'_{i,n-1},\quad b'=\sum_{i=1}^{n-1} m'_{i,n-1}-\sum_{i=1}^{n-1} m_{i,n-1}$$

S is given in Eq. (3.8).

It is then found that the contraction process goes through for all IU(n), because the terms containing infinity all cancel out. Therefore, the representation functions of IU(n) can be obtained explicitly from those of U($n+1$) as given in Eq. (5.1) by omitting all factors containing m_{1n+1} and $m_{n+1,n+1}$, and replacing $\cos\theta$ by 1 and $\sin\theta$ by $\kappa\xi$. The final result of the representation function of IU($n-1$) is

$${}^{I}d^{\kappa m_{2n}\cdots m_{n-1,n}}_{\substack{[m]_{n-1}[m']_{n-1}\\ [m]_{n-2}[m]_{n-2}}}(\xi)=\frac{\mathfrak{N}([m]_n)}{[\mathfrak{M}([m]_{n-1})\mathfrak{M}([m']_{n-1})]^{1/2}}\;\frac{T_{n,n-1}([m]_n,[m]_{n-1})T_{nn}{}^2([m]_n,[m]_n)T_{n,n-1}([m]_n,[m']_{n-1})}{S_{n,n-1}([m'']_{n-1},0;[m]_{n-1})S_{n,n-1}([m'']_{n-1}0;[m']_{n-1})}$$
$$\times\frac{S^2_{n-1,n-2}([m'']_{n-1},[m]_{n-2})S^2_{n-1,n-1}([m'']_{n-1}[m'']_{n-1})}{T^2_{nn}([m]_n;[m'']_{n-1},0)S_{n-1,n-2}([m]_{n-1}[m]_{n-2})S_{n-1,n-2}([m']_{n-1}[m]_{n-2})}$$
$$\times\frac{1}{S_{n-1,n-1}([m'']_{n-1},[m]_{n-1})S_{n-1,n-1}([m'']_{n-1},[m']_{n-1})}(\kappa\xi)^{2\Sigma[m'']_{n-1}-\Sigma[m']_{n-1}-\Sigma[m]_{n-1}},$$

where $\mathfrak{N}$ and T are obtained from $\mathfrak{M}$ and S respectively by omitting all factors containing m_{1n} and m_{nn}. The summation over m''_{1n-1} is an infinite sum, while the summation over the other indices are finite in accordance with the branching rules of U(n). Again, we find that (5.4) has the following two properties: (1) It is convergent for all values of κ,ξ. (2) It can be expressed as a sum over a generalized hypergeometric function ${}_{3(n-2)}F_{3n-5}$.

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Super Lie groups: global topology and local structure

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A general mathematical framework for the super Lie groups of supersymmetric theories is presented. The definition of super Lie group is given in terms of supermanifolds, and two theorems (analogous to theorems in classical Lie group theory) are proved. The relationship of the super Lie groups defined here to the formal groups of Berezin and Kac and the graded Lie groups of Kostant is analyzed.

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1. INTRODUCTION

Several recent theories, notably supersymmetry,[1] supergravity[2] and also superunified theories of weak and electromagnetic interactions[3] have considered multiplets of fields transforming under a rule which is expressed infinitesimally by a graded Lie algebra with infinitesimal Grassmann parameters. The assumption is that the graded Lie algebra is the algebra of infinitesimal generators of some "super Lie group"; such groups have been constructed by exponentiation of the algebra using the Baker–Campbell–Hausdorff formula,[4] or exponentiation of matrix representations of the algebra.[5] The nature of the infinitestimal parameters suggests that a global super Lie group should be a space with local coordinates in a Grassmann algebra, i.e., a supermanifold, and thus one is led naturally, by analogy with the definition of a conventional Lie group, to a definition of a super Lie group as a group which is also a supermanifold,[6] with superanalytic group operation. This approach is explored in detail in this paper, and provides a general mathematical framework for the groups mentioned above. The graded Lie algebra of infinitesimal generators of a super Lie group appears in a manner exactly analogous to the Lie algebra of infinitesimal generators of a conventional Lie group. The supermanifolds used in this definition are those of Ref. 6; because such a supermanifold is a topological space, the formulation of super Lie groups given here naturally includes global topological properties. It should now be possible to consider whether or not the global properies of super Lie groups have physical implications analogous to those of conventional Lie groups.

Super Lie groups derived from graded Lie algebras were first considered by Berezin and Kac, in a mathematical context, some years before the physical theories mentioned above; in their paper "Lie groups with commuting and anticommuting parameters,"[7] they give a definition of a formal (super) Lie group. Subsequently Kostant has given a definition of a graded Lie group.[8] Neither the formal groups of Berezin and Kac nor the graded Lie groups of Kostant are actually abstract groups, unlike the super Lie groups defined in this paper. These super Lie groups bear the same relationship to the formal groups of Berezin and Kac as do conventional Lie groups to the formal Lie groups first introduced by Bochner.[9] The graded Lie groups of Kostant can be included in the super Lie group formulation given here in a natural way (as is explained in Sec. 6 of this paper).

Section 2 of this paper contains the definition of a super Lie group. In Sec. 3 it is proved that the left invariant vector fields on a super Lie group form a "graded Lie module" (an extension of the concept of graded Lie algebra), while Sec. 4 contains several examples of super Lie groups and their corresponding graded Lie modules. In Sec. 5 it is proved that, corresponding to any graded Lie module, there is at least one super Lie group, and a means of identifying all super Lie groups with some specified graded Lie module is given; thus the problem of classifying super Lie groups is reduced to the problem of classifying graded Lie modules. In Sec. 6 it is shown how the set of Kostant graded Lie groups can be identified with a subset of the set of super Lie groups in a precise and natural way.

In this paper attention is confined to real super Lie groups, that is, the Grassmann algebras and graded Lie algebras used are all algebras over the real numbers. Extension to algebras over the complex numbers is possible. Notation required for certain algebraic results in Secs. 3.5 and 3.6 is defined in the Appendix.

2. THE DEFINITION OF A SUPER LIE GROUP

The parameters of the infinitesimal transformations indicate the nature of the local coordinates of a super Lie group: when the graded Lie algebra of infinitesimal transformations is (m,n)–dimensional, the parameters are m even and n odd elements of a Grassmann algebra, and thus a space with this type of local coordinate, i.e., an (m,n)–dimensional supermanifold, is suggested. The definition of a super Lie group is a straightforward generalization of the definition of a conventional Lie group.

Definition 2.1: An (m,n)–dimensional super Lie group is a set H such that

(a) the set H is an abstract group,

(b) the set H is an (m,n)—dimensional superanalytic supermanifold,

(c) the mapping $(h_1,h_2)\rightarrow h_1 h_2^{-1}$ of the product supermanifold $H\times H$ into H is superanalytic.

Here the definition of supermanifold and superanalytic are those given in Ref. 6, briefly summarized below. ($B_L{}^{m,n}$ denotes the Cartesian product of m copies of the even part and n copies of the odd part of B_L, the Grassmann algebra over $\mathbb{R}^L$.)

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Definition 2.2: An (m,n)–dimensional superanalytic supermanifold over B_L is defined to be a Hausdorff topological space Y together with a set of charts $\{(U_\alpha,\psi_\alpha)\}$ such that

(a) $\cup_\alpha U_\alpha = Y$,

(b) each ψ_α is a homeomorphism of U_α onto an open subset of $B_L^{m,n}$,

(c) the functions $\psi_\alpha \circ \psi_\beta^{-1}:\psi_\beta(U_\alpha \cap U_\beta) \to \psi_\alpha(U_\alpha \cap U_\beta)$ are superanalytic, where in (b) the topology on $B_L^{m,n}$ is the usual toplogy on $B_L^{m,n}$ regarded as a finite-dimensional vector space, and in (c), if U is open in $B_L^{m,n}$, then $f:U \to B_L$ is said to be superanalytic on U if, given any $p = (p_1,...,p_{m+n})$ in U, there exists a neighborhood N of p such that, for all q in N, $f(q)$ is equal to the sum of an absolutely convergent power series of this form:

$$f(q) = \sum_{k_1=0,...,k_{m+n}=0}^{\infty} a_{k_1 \cdots k_{m+n}} (q_1 - p_1)^{k_1} \cdots (q_{m+n} - p_{m+n})^{k_{m+n}} \tag{2.1}$$

(with each $a_{k_1 \cdots k_{m+n}}$ an element of B_L).

The concept of superanalyticity can then be extended to maps between manifolds, via charts, in the usual way.

In Ref. 6, B_∞, an infinite-dimensional analogue of B_L was defined, so that it is possible to define supermanifolds and super Lie groups over an infinite dimensional Grassmann-type algebra.

For future reference, some definitions and results originally given in Ref. 6 are summarized here.

Definition 2.3: (a) If U is, open in $B_L^{m,n}$ and $f:U \to B_L$, f is said to be "G^∞" on U if, given $(a_1,...,a_{m+n})$ and $(a_1 + h_1,...,a_{m+n} + h_{m+n})$ in U,

$$f(a_1 + h_1,...,a_{m+n} + h_{m+n}) = f(a_1,...,a_{m+n}) + \sum_{k=1}^{m+n} h_k G_k f(a_1,...,a_{m+n}) + O\,\|(h_1,...,h_{m+n})\|^2, \tag{2.2}$$

where the partial derivatives $G_k f$ are in turn G^∞ functions of U into B_L.

(b) If V is an open subset of a supermanifold Y, then $G^\infty(V)$ denotes the set of G^∞ functions of V into B_L, [i.e., functions $f:V \to B_L$ such that $f \circ \psi_\alpha^{-1}:\psi_\alpha(V \cap U_\alpha) \to B_L$ is G^∞ for any chart (U_α,ψ_α)].

Proposition 2.4: $G^\infty(V)$ is a graded commutative algebra and a graded left B_L–module.

Definition 2.5: A vector field on V is a vector space endomorphism X of $G^\infty(V)$ such that, given f,g in $G^\infty(V)$ and b in B_L,

$$\left.\begin{aligned} X(fg) &= (Xf)g + (-1)^{|X||f|} fXg \\ X(bg) &= (-1)^{|b||X|} bXg, \end{aligned}\right\} \tag{2.3}$$

(where $|X|$, $|f|$ and $|b|$ represents the degree of X, f, and b, respectively).

In view of the similarity between Lie groups and super Lie groups, many of the results of conventional Lie group theory extend to analogous results in super Lie group theory. as will emerge in succeeding sections.

3. THE GRADED LIE MODULE OF A SUPER LIE GROUP

It is a well known result of classical Lie group theory that the left (or right) invariant vector fields [sometimes referred to as infinitesimal right (or left) translations] form a Lie algebra. The analogous result for super Lie groups is that the left invariant vector fields form a "graded Lie module."

Definition 3.1: A graded Lie left B_L–module is a graded Lie algebra W (over $\mathbb{R}$) which is also a graded left B_L–module such that

$$[bX_1,X_2] = b\,[X_1,X_2] \tag{3.1}$$

for all b in B_L, X_1, X_2 in W.

Definition 3.2: A graded B_L–module is said to have dimension (m,n) if it is a free module with a basis consisting of m even and n odd elements. (It can be shown that the dimension is well defined.)

Many, but not all, of the graded Lie modules considered in this paper are of the form $W = B_L \otimes_{\mathbb{R}} \mathbf{g}$ where $\mathbf{g}$ is a graded Lie algebra over the real numbers,

$$[(a \otimes X),(b \otimes Y)] := (-1)^{|b||X|} ab \otimes [X,Y] \tag{3.2}$$

and

$$a(b \otimes Y) := ab \otimes Y$$

(for all a, b in B_L and X,Y in $\mathbf{g}$).

If $\mathbf{g}$ is an (m,n)–dimensional graded Lie algebra, then $B_L \otimes_{\mathbb{R}} \mathbf{g}$ is an (m,n)–dimensionl graded Lie left B_L–module. If $W \simeq B_L \otimes_{\mathbb{R}} \mathbf{g} \simeq B_L \otimes_{\mathbb{R}} \mathbf{g}'$ then $\mathbf{g} \simeq \mathbf{g}'$, so that the decomposition is unique.

Definition 3.3: (a) Let H be a super Lie group and $h \in H$. Define

$$\delta_h:H \to H \text{ by } \delta_h(h') := hh' \text{ for all } h' \in H. \tag{3.3}$$

(As a direct consequence of the definition of a super Lie group, δ_h must be superanalytic.)

(b) Define δ_{h*} to be the induced mapping of vector fields on H, i.e.,

$$\delta_{h*}(X)f = X(f \circ \delta_h) \text{ for all } f \text{ in } G^\infty(H). \tag{3.4}$$

(c) A vector field X on H is said to be "left invariant" if $\delta_{h*}X = X$ for all h in H.

Equipped with this definition, the proof of the main theorem of this section proceeds very much as in the classical case.

Theorem 3.4: Let $\mathscr{L}(H)$ denote the set of left invariant vector fields on an (m,n)–dimensional super Lie group over B_L. Then $\mathscr{L}(H)$ is an (m,n)–dimensional graded Lie left B_L–module with bracket operation

$$\begin{aligned} &[,]:\mathscr{L}(H) \times \mathscr{L}(H) \to \mathscr{L}(H) \\ &[X,Y] := XY - (-1)^{|X||Y|} YX, \quad X,Y \in \mathscr{L}(H). \end{aligned} \tag{3.5}$$

Outline of proof: It is proved in Ref. 6 that the set of vector fields on H forms a graded Lie left B_L–module under the bracket operation defined above. That $\mathscr{L}(H)$ is a subgraded Lie left B_L–module [in particular that $\mathscr{L}(H)$ is closed under the bracket operation] can be proved exactly as in the classical case.

Let $T_e(H)$ be the analogue of the tangent space at the identity e of H (i.e., $T_e(H)$ is the set of maps $X_e:G^\infty(e) \to B_L$ such that $X_e(fg) = (X_e f)g(e) + (-1)^{|X||f|} f(e) X_e g$.) Then $T_e(H)$ can be shown to be a graded left B_L–module of dimension (m,n) (cf. Ref. 6, proposition 5.9). Also $\mathscr{L}(H)$ can be shown to be isomorphic (*qua* left B_L-module) to $T_e(H)$ exactly as in the classical case.

In the case where L is finite, an (m,n)–dimensional superanalytic supermanifold Y over B_L is also a $2^{L-1}(m+n)$–dimensional real analytic manifold, and a superanalytic mapping of $Y \times Y \to Y$ where Y is regarded as a supermanifold is *a fortiori* an analytic mapping when Y is considered merely as a manifold. Thus an (m,n)–dimensional super Lie group over B_L is also a $2^{L-1}(m+n)$–dimensional real Lie group.

The next proposition establishes a relationship between the graded Lie module of a super Lie group H and the Lie algebra of H regarded simply as a Lie group. It should be noted that if W is an (m,n)–dimensional graded Lie left B_L–module then, (since the even and odd parts of B_L are both 2^{L-1}–dimensional vector spaces) the even part of W can be regarded as a $2^{L-1}(m+n)$–dimensional vector space, and, as such, becomes a $2^{L-1}(m,n)$–dimensional real Lie algebra. A rather heavy-handed method, employing local coordinates, is used in the proof of this proposition because it introduces notation useful in subsequent sections.

Proposition 3.5: Let H be an (m,n)–dimensional super Lie group over B_L (where $n \leqslant L < \infty$) and let W be its graded Lie module. Further, let $\mathbf{h}$ be the $2^{L-1}(m+n)$–dimensional Lie algebra of H regarded as a $2^{L-1}(m+n)$–dimensional real Lie group. Then the even part of W (regarded as a $2^{L-1}(m+n)$–dimensional Lie algebra) is isomorphic to $\mathbf{h}$.

Proof: Let V be a coordinate neighborhood of H containing the identity e of H, and V' be an open neighborhood of e such that $V'V' \subset V$. Let $\psi_e: V \to B_L{}^{m,n}$ be superanalytic coordinates on V with $\psi_e(e) = 0$ and define

$$\mathbf{K}: \psi_e(V') \times \psi_e(V') \to \psi_e(V) \qquad (3.6)$$

by

$$\mathbf{K}(\psi_e(h_1);\psi_e(h_2)) := \psi_e(h_1h_2) \quad \forall h_1,h_2 \in V'.$$

Let $\mathbf{K}^i$, ψ_e^i denote the ith component of $\mathbf{K}$, ψ_e respectively for $i = 1,\ldots,m+n$. Finally, define

$$\chi^i_j: \psi_e(V') \to B_L \quad i,j = 1,\ldots,m+n$$

by

$$\chi^i_j(x_1,\ldots,x_{m+n}) := G_{j(y)}\mathbf{K}^i(x_1,\ldots x_{m+n};y_1,\ldots,y_{m+n})|_{y=0} \qquad (3.7)$$

and

$$X_i: G^\infty(V') \to G^\infty(V') \qquad (3.8)$$

by

$$X_i f := \sum_{j=1}^{m+n} [\chi^j_i G_j(f \cdot \psi_e{}^{-1})] \circ \psi_e.$$

(For the definition of the partial derivatives G_j, cf. Def. 2.3.) A straightforward adaptation of the classical proof,[10] using the chain rule for differentiation of functions of $B_L{}^{m,n}$ [cf. Ref. 6 Proposition 2.12(g)] shows that $\{X_i | i = 1,\ldots,m+n\}$ forms a basis of $\mathscr{L}(H)$, the graded Lie module of H. Also, if elements C^k_{ij} of B_L $(i,j,k = 1,\ldots,m+n)$ are defined by $[X_i,X_j] = C^k_{ij}X_k$, then

$$C^k_{ij} = G_i\chi^k_j(0) - (-1)^{|i||j|}G_j\chi^k_i(0). \qquad (3.9)$$

(The rest of the proof makes use of the notation defined in the Appendix.)

Define analytic coordinates $\phi e_{V'} \to \mathbb{R}^{2^{L-1}(m+n)}$ by $\phi_e := \iota \circ \psi_e$. Also, define

$$\kappa: \phi_e(V') \times \phi_e(V') \to \phi_e(V)$$

by

$$\kappa(\phi_e(h_1);\phi_e(h_2)) := \phi_e(h_1h_2) \quad \forall h_1,h_2 \in V'. \qquad (3.10)$$

Let $\phi^{i\mu}{}_e, \kappa^{i\mu}$ be the $(i\mu)$ components of ϕ_e, κ, respectively, and define

$$\chi^{i\mu}_{j\nu}: \phi_e(V') \to \mathbb{R}$$

by

$$\chi^{i\mu}_{j\nu}(x) := \left.\frac{\partial \kappa^{i\mu}(x,y)}{\partial y^{j\nu}}\right|_{y=0}.$$

Then the set $\{X_{i\mu} | i = 1,\ldots,m+n; \mu \in M_{L,|i|}\}$ with $X_{i\mu} := \chi^{j\nu}_{i\mu}\partial_{j\nu}$ forms a basis of $\mathbf{h}$, the Lie algebra of H regarded as a Lie group.

Also, if

$$[X_{i\mu}, X_{j\nu}] = \sum_{k=1}^{m+n} \sum_{\rho \in M_{L,|k|}} B^{k\rho}_{i\mu j\nu} X_{k\rho}$$

then

$$B^{k\rho}_{i\mu j\nu} = \partial_{i\mu}\chi^{k\rho}_{j\nu}(0) - \partial_{j\nu}\chi^{k\rho}_{i\mu}(0).$$

Expanding $\mathbf{K}(x,y)$ and $\kappa(x,y)$ as power series about zero shows that, if $C^k_{ij} = C^{k\tau}_{ij}\beta_\tau$, where $C^{k\tau}_{ij} \in \mathbb{R}$, then

$$B^{k\rho}_{i\mu j\nu} = C^{k\tau}_{ij} F^\alpha_{\nu\mu} F^\rho_{\alpha\tau} \qquad (3.11)$$

(cf. Appendix for notation).

But $\{\beta_\mu X_i | i = 1,\ldots,m+n, \mu \in M_{L,|i|}\}$ is a basis of the even part of the graded Lie module of H (regarded as a $2^{L-1}(m+n)$–dimensional Lie algebra) and

$$\begin{aligned}[\beta_\mu X_i, \beta_\nu X_j] &= (-1)^{|i||\nu|}\beta_\mu\beta_\nu[X_i,X_j] \\ &= \beta_\nu\beta_\mu C^{k\rho}_{ij}\beta_\rho X_k \\ &= B^{k\rho}_{i\mu j\nu}\beta_\rho X_k. \end{aligned}$$

■

4. EXAMPLES OF SUPER LIE GROUPS

In this section several examples of super Lie groups and their graded Lie modules are described.

Examples 4.1: The Abelian super Lie groups.

(a) $B_L{}^{m,n}$ itself, with the additive part of its vector space structure, is an (m,n)–dimensional Abelian super Lie group with Abelian graded Lie module.

(b) As in the case of Lie groups, factorization by appropriate discrete subgroups gives super Lie groups homeomorphic to $\mathbb{R}^{2^{L-1}(m+n)-k} \times (S^1)^k$, [for $0 \leqslant k \leqslant 2^{L-1}(m+n)$] isomorphic qua Lie groups to $\mathbb{R}^{2^{L-1}(m+n)-k} \otimes (U(1))^k$. (The existence of such super Lie groups follows from theorem 5.5.)

Example 4.2: Two non-Ableian super Lie groups with the same graded Lie module, but topologically distinct in the odd as well as the even sector. (Cf. Appendix for definition of the β_μ.)

(a) $H = B_4{}^{1,1} = B_{4,0} \times B_{4,1}$, with group operation defined by

$$(a,b) \circ (c,d) := (a + c + \tfrac{1}{2}\beta_1\beta_2 bd, b + d).$$

Topologically, H is homeomorphic to $\mathbb{R}$.[8] The graded Lie module of H is $\{X_1, X_2\}$ with X_1 even, X_2 odd and

$$[X_1, X_1] = [X_1, X_2] = 0. \quad [X_2, X_2] = \beta_1\beta_2 X_1.$$

It should be noted that this graded Lie module cannot be expressed as the tensor product of B_4 with a graded Lie algebra.

(b) Let $K := H/D$ where D is the discrete, central subgroup of H consisting of elements of the form

$$\Big(\sum_{\mu \in \mu_{4,0}} m^\mu \beta_\mu, n^{(1)}\beta_1 + n^{(2)}\beta_2 + n^{(123)}\beta_1\beta_2\beta_3 + n^{(134)}\beta_1\beta_3\beta_4 + n^{(124)}\beta_1\beta_2\beta_4 + n^{(234)}\beta_2\beta_3\beta_4 \Big),$$

where the m^μ, n^μ are integers. K is then a super Lie group with the same graded Lie module but now homeomorphic to $(S^1)^6 \times \mathbb{R}^2$.

Example 4.3: The supersymmetry group.[4] This is $B_L^{4,4}$ with group operation defined by

$$(x^\mu, \theta^\alpha) \circ (y^\mu, \epsilon^\alpha) := (x^\mu + y^\mu - \tfrac{1}{2} i \bar\theta \gamma^\mu \epsilon, \epsilon^\alpha + \theta^\alpha)$$

[with the notation of Ref. (4)] and graded Lie module $B_L \otimes \mathbf{g}$ where $\mathbf{g}$ is the (4,4)–dimensional graded Lie algrebra of supersymmetry.

Example 4.4: The graded extension of the Poincaré group. This is the semi-direct product of a Lie group (the Lorentz group) with a super Lie group (the supersymmetry group) where, given Γ, Λ in the Lorentz group and (x^μ, θ^α), (y^μ, ϵ^α) in the supersymmetry group,

$$(\Lambda, (x^\mu, \theta^\alpha)) \circ ((\Gamma, (y^\mu, \epsilon^\alpha)) := (\Lambda\Gamma, (x^\mu, \theta^\alpha) \circ (a(\Gamma) y^\mu, b(\Gamma) \epsilon^\alpha)), \tag{4.1}$$

where a and b are the standard vector and spinor representations of the Lorentz group.

5. THE SUPER LIE GROUPS WHICH CORRESPOND TO A GIVEN GRADED LIE MODULE

It was proved in Sec. 3 that the set of left invariant vector fields on a super Lie group form a graded Lie module. In this section the converse problem is considered and it is proved (Theorem 5.5) that, given an arbitrary (m,n)–dimensional graded Lie left B_L–module W (with L finite), there always exists a super Lie group whose graded Lie module is W; in fact, it is established that any real Lie group with Lie algebra equal to the even part of W (regarded as a Lie algebra) can be given the structure of a super Lie group with graded Lie module W. Combining this with Proposition 3.5 shows that the set of super Lie groups with graded Lie module W exactly coincides with the set of Lie groups with Lie algebra equal to the even part of W. Thus the problem of classifying all super Lie groups over a finite-dimensional Grassmann algebra B_L is reduced to that of classifying all graded Lie left B_L–modules; it seems likely that a suitable limiting process would extend this result to super Lie groups over the infinite–dimensional algebra B_∞.

The first step in proving the main theorem is to develop a criterion by which it may be determined whether or not a given analytic function of $\mathbb{R}^{2^{L-1}(m+n)}$ is a superanalytic function of $B_L^{m,n}$.

Lemma 5.1: Suppose $f: U \to B_L$ is analytic on some neighborhood U of $\mathbf{0}$ in $\mathbb{R}^{2^{L-1}(m+n)}$. Then, with the notation defined in the Appendix, $f \circ \iota: \iota^{-1}(U) \to B_L$ is superanalytic on $\iota^{-1}(U)$ if and only if there exist, for each sequence of integers $(p_1, \ldots, p_k)$ in N_{m+n}, elements $f_{p_1 \cdots p_k}$ of B_L such that

$$\partial_{p_k \sigma_k} \cdots \partial_{p_1 \sigma_1} f(0) = \beta_{\sigma_1} \cdots \beta_{\sigma_k} f_{p_1 \cdots p_k}, \tag{5.1}$$

where each σ_i, $i = 1, \ldots, k$ is an arbitrary element of M_{L, p_i}.

Indication of proof: This Lemma is easily proved by considering the series expansion of f about zero.

Corollary 5.2:

$$f_{p_1 \cdots p_k} = G_{p_k \cdots p_1} f(0). \tag{5.2}$$

The next Lemma shows how, given a Lie group with Lie algebra equal to the even part of a graded Lie module, the local analytic structure of this Lie group may be used to construct a local superanalytic structure.

Lemma 5.3: Let W be an (m,n)–dimensional graded Lie left B_L module (where $n \leqslant L < \infty$) and $\{X_i | i = 1, \ldots, m+n\}$ be a basis of W (with X_i even for $i = 1, \ldots, m$ and X_i odd for $i = m+1, \ldots, m+n$). Also let $\mathbf{h}$ be the $2^{L-1}(m+n)$–dimensional real Lie algebra derived from the even part of W; (then $\mathbf{h}$ has a basis

$$\{X_{i\mu} | X_{i\mu} := \beta_\mu X_i, \quad i = 1, \ldots, m+n, \quad \mu \in M_{L,|i} \}.)$$

Suppose that H is a Lie group with Lie algebra $\mathbf{h}$, and that $\phi_e: V \to \mathbb{R}^{2^{L-1}(m+n)}$ are canonical coordinates (with respect to the basis $X_{i\mu}$ of $\mathbf{h}$) on some neighborhood V of the identity e of H. Let U be a neighborhood of e such that $UU \subset V$ and let $\kappa: \phi_e(U) \times \phi_e(U) \to \phi_e(V)$ be the analytic function defined by

$$\kappa(\phi_e(g); \phi_e(h)) := \phi_e(gh) \quad \forall g, h \in U, \tag{5.3}$$

[with $(i\mu)$ component denoted $\kappa^{i\mu}$].

Also let $\psi_e: V \to B_L^{m,n}$ with

$$\psi_e := \iota^{-1} \circ \phi_e. \tag{5.4}$$

Then, if $\mathbf{K}: \psi_e(u) \times \psi_e(u) \to \psi_e(V)$ is defined by

$$\mathbf{K}^i(x) := \sum_{\mu \in M_{L,|i}} \kappa^{i\mu}(\iota(x)) \beta_\mu, \tag{5.5}$$

(a) $\mathbf{K}(\psi_e(g); \psi_e(h)) = \psi_e(gh)$ for all g, h in U;

(b) $\mathbf{K}$ is superanalytic on $\psi_e(U) \times \psi_e(U)$,

(i.e., group operations expressed in terms of the chart (V, ψ_e) are superanalytic).

Further, if $\chi^i_j: \psi_e(U) \to B_L$ is defined by

$$\chi^i_j(x) := G_{j(y)} \mathbf{K}^i(x;y)|_{y=0} \quad i,j = 1, \ldots, m+n, \tag{5.6}$$

and $C^k_{ij}(x)$ $(i,j,k = 1, \ldots, m+n)$ are elements of B_L such that $[X_i, X_j] = C^k_{ij} X_k$, then $G_i \chi^k_j(0) = \tfrac{1}{2} C^k_{ij}$.

Outline of proof:

(a) This result follows immediately from Eqs. (5.3), (5.4), and (5.5).

(b) Let

$$\chi^{i\mu}_{j\nu}(x) := \left. \frac{\partial \kappa^{i\mu}(x,y)}{\partial y^{j\nu}} \right|_{y=0}, \tag{5.7}$$

where $x, y \in \phi_e(V)$.

Then, using induction and Lie's first theorem, it may be proved that

$$\frac{\partial \kappa^{i\mu}(x,y)}{\partial y^{p_k\sigma_k}\cdots\partial y^{p_1\sigma_1}} = \sum_{\tau_i\in M_{L|S_i|}} T(k)^{a\beta_1\cdots\beta_k}_{S_1\cdots S_k} F^{\alpha}_{\tau_1\cdots\tau_k\beta_k\cdots\beta_1} \times \chi^{i\mu}_{a\alpha}(\kappa(x,y))\widetilde{\chi}^{S_1\tau_1}_{p_1\sigma_1}(y)\cdots\widetilde{\chi}^{S_k\tau_k}_{p_k\sigma_k}(y) \quad (5.8)$$

for all $(p_1,\ldots,p_k)$ in N_{m+n} and σ_i in $M_{L|p_i|}$ $(i = 1,\ldots,k)$ (with the $T(k)^{a\beta_1\cdots\beta_k}_{S_1\cdots S_k}$ somewhat involved combinations of the elements $C^{k\tau}_{ij}$ in $\mathbb{R}$ such that $C^k_{ij} = C^{k\tau}_{ij}\beta_\tau$). Now let

$$\kappa^i_{p_1\cdots p_k}(x) := \sum_{\substack{\eta_1\in M_{L,|P_1|}\\ \cdots \\ \eta_k\in M_{L,|P_k|}}} \left.\frac{\partial \kappa^{i\mu}(x,y)}{\partial y^{P_1\eta_1}\cdots\partial y^{P_k\eta_k}}\right|_{y=0} \times A^{\eta_1\tau_1}_{\mu} A^{\eta_2\tau_2}_{\tau_1}\cdots A^{\eta_k\tau_k}_{\tau_{k-1}}\beta_{\tau_k}. \quad (5.9)$$

Then it can be proved [using Eqs. (5.8), (A2), and (A3)] that

$$\frac{\partial \mathbf{K}^i(x,0)}{\partial y^{P_1\sigma_1}\cdots\partial y^{p_k\sigma_k}} = \beta_{\sigma_1}\cdots\beta_{\sigma_k}\kappa^i_{P_1\cdots P_k}(x), \quad (5.10)$$

and thus, by Lemma 5.1, $\mathbf{K}$ is superanalytic in y. Similarly it can be shown that $\mathbf{K}$ is superanalytic in x.

(c) By Corollary 5.2 and Eq. (5.9)

$$\chi^i_j(x) = \chi^{i\mu}_{j\nu}(x)A^{\nu\alpha}_{\mu}\beta_\alpha .$$

Hence

$$\partial_{k\rho}\chi^i_j(0) = \partial_{k\rho}\chi^{i\mu}_{j\nu}(0)A^{\nu\alpha}_{\mu}\beta_\alpha = \tfrac{1}{2}\beta_\rho C^i_{kj},$$

[using Eqs. (3.11), (A2), and (A3)], and thus, again by Corollary 5.2,

$$G_k\chi^i_j(0) = \tfrac{1}{2}C^i_{kj}. \quad ■$$

It is next shown, in Lemma 5.4, that a topological group with a local superanalytic structure on a neighborhood of the identity can be given a (unique) global superanalytic structure making it into a super Lie group.

Lemma 5.4: Let G be a topological group and suppose there is a neighborhood V of the identity e of G on which is defined a homeomorphism $\psi_e: V \to B_L^{m,n}$ of V onto an open subset of $B_L^{m,n}$. Then, if the product in G is superanalytic when expressed in terms of this chart, G can be defined in just one way as a super Lie group such that the given chart, when restricted to a suitable nucleus, belongs to the superanalytic structure of G. The topology on G (qua super Lie group) then coincides with the given topology on G.

Outline of proof: Let W_1, W_2, be neighborhoods of e such that $W_1W_2 \subset V$ and $W_1W_2^{-1} \subset W_1$. Then the global superanalytic structure on G may be defined by the set of charts

$$\{(V_g,\psi_g)|g\in G\} \quad \text{where} \quad V_g := W_2 g$$

and

$$\psi_g(kg) := \psi_e(k) \quad \forall k\in W_2. \quad (5.11)$$

(The proof that this set of charts does give G the structure of a super Lie group is a straightforward generalization of the classical proof.[10])

■

Theorem 5.5: Let W be an (m,n)–dimensional graded Lie left B_L module, and let $\mathbf{h}$ be the $2^{L-1}(m+n)$–dimensional real Lie algebra derived from the even part of W. Let H be any $2^{L-1}(m+n)$–dimensional real Lie group with Lie algebra $\mathbf{h}$. Then H can be given the structure of an (m,n)–dimensional super Lie group over B_L with graded Lie module W.

Proof: Lemmas 5.3 and 5.4 together imply that H can be given the structure of a super Lie group. Also, with the notation of Lemma 5.3, if $X_i := \chi^j_i(x)G_j$ $i = 1,\ldots,m+n$, then $\{X_i | i = 1,\ldots,m+n\}$ is a basis of the graded Lie module of H (cf proposition 3.5). Hence if

$$[X_i,X_j] = D^k_{ij}X_k ,$$

then

$$D^k_{ij} = G_j\chi^k_i(0) - (-1)^{|i||j|}G_j\chi^k_j(0) = C^k_{ij}.$$

Thus the graded Lie module of H is equal to W.

■

6. SUPER LIE GROUPS AND GRADED LIE GROUPS

A definition of graded manifold and graded Lie group has been given by Kostant.[8] In a previous paper[6] it has been shown how the set of (m,n)–dimensional graded manifolds can be identified with a subset of the set of (m,n)–dimensional G^∞ supermanifolds over B_L (for any finite L not less than n) in a very precise and natural way. In this section it is shown that, where a graded manifold (G,A) is a graded Lie group, with graded Lie algebra $\mathbf{g}$, the associated supermanifold over B_L can be given the structure of a super Lie group, with graded Lie module $B_L \otimes \mathbf{g}$.

This result is achieved in three stages:

I. The supermanifold $K(G,A)$ associated with the graded Lie group (G,A) is constructed according to the method of Ref. 6.

II. A super Lie group H over B_L, with graded Lie module $B_L \otimes \mathbf{g}$, is constructed.

III. H and $K(G,A)$ are shown to be super diffeomorphic, so that $K(G,A)$ becomes a super Lie group with graded Lie module $B_L \otimes \mathbf{g}$.

Full details of Kostant's definition of graded Lie group may be found in Ref. 8. The following properties of graded Lie groups will be required here:

(a) If (G,A) is an (m,n)–dimensional graded Lie group, then G is an m–dimensional Lie group and A is a sheaf of graded algebras over G with $A(U) \simeq C^\infty(U)\otimes B_n$ for all U open in G.

(b) Associated with (G,A) is an (m,n)–dimensional graded Lie algebra $\mathbf{g} = \mathbf{g}_0 \oplus \mathbf{g}_1$, with $\mathbf{g}_0$ (the even part of $\mathbf{g}$) equal to the Lie algebra of G.

(c) There exists a smooth representation

$$\pi: G \to (\mathrm{aut}\,\mathbf{g})_0 \quad \text{such that} \quad \pi|_{G_e} = \mathrm{Ad}_{\mathbf{g}}, \quad (6.1)$$

where G_e is the identity component of G and $\mathrm{Ad}_{\mathbf{g}}$ is the exponentiation of

$$\mathrm{ad}_{\mathbf{g}}: \mathbf{g}_0 \to \mathrm{end}\,\mathbf{g}$$
$$\mathrm{ad}_{\mathbf{g}}(X)(Z) := [X,Z] \quad \forall X\in\mathbf{g}_0,\ Z\in\mathbf{g}. \quad (6.2)$$

Throughout the remainder of this section, (G,A) is an arbitrary (m,n)–dimensional graded Lie group with graded Lie algebra $\mathbf{g} = \mathbf{g}_0 \oplus \mathbf{g}_1$, and L is a finite integer not less than n.

I. An atlas can be defined on G as follows: Let V, U, U_1, be connected coordinate neighborhoods of the identity e of G such that $UU \subset V$ and $U_1 U_1^{-1} \subset U$. Let $\phi_e : U_1 \to \mathbb{R}^m$ be an analytic chart on U_1, canonical with respect to a basis $\{X_i | i = 1,...,m\}$ of $\mathbf{g}_0$. Define

$$U_g := U_1 g \quad \forall g \in G$$

and

$$\phi_g : U_g \to \mathbb{R}^m, \qquad \phi_g(xg) := \phi_e(x) \quad \forall x \in U_1. \tag{6.3}$$

then $\{(U_g, \phi_g)\}$ forms an atlas on G compatible with the Lie group structure on G.[10]

Now let ϵ be the augmentation map which projects elements of $B_L{}^{m,n}$ onto their non-nilpotent parts, i.e.,

$$\epsilon : B_L{}^{m,n} \to \mathbb{R}^m,$$

$$\epsilon\Big(\sum_{\mu \in M_{L,0}} a^1_\mu \beta_\mu, ..., \sum_{\mu \in M_{L,0}} a^m_\mu \beta_\mu, b^1, ..., b^n\Big) := (a^1_\Omega, ..., a^m_\Omega). \tag{6.4}$$

Also, given U open in $\mathbb{R}^m$ and f a C^∞ function of U into $\mathbb{R}$, define the G^∞ function

$$Z(f) : \epsilon^{-1}(U) \to B_L$$

by

$$Z(f)(a^1,...,a^{m+n}) := \sum_{i_1 = 0 ... i_m = 0}^{L} \frac{1}{i_1! \cdots i_m!} (\partial_1^{i_1} ... \partial_m^{i_m} f)(\epsilon(a)) \times (a^1 - \epsilon(a^1)1)^{i_1} \cdots (a^m - \epsilon(a^m)1)^{i_m}. \tag{6.5}$$

Then the supermanifold $K(G,A)$ constructed from the graded Lie group (G,A) by the method of Ref. 6 may be most simply characterised as an (m,n)-dimensional supermanifold Y over B_L which possesses a chart $\{(V_g, \psi_g) | g \in G\}$ such that $\psi_g(V_g) = \epsilon^{-1}(\phi_g(U_g))$ and the functions

$$\psi_g \circ \psi_{g'}^{-1} : \psi_{g'}(V_g \cap V_{g'}) \to \psi_g(V_g \cap V_{g'})$$

satisfy

$$\left.\begin{array}{ll} \psi^i_g \circ \psi_{g'}^{-1} = Z(\phi^i_g \circ \phi_{g'}^{-1}) & i = 1,...,m \\ \psi^i_g \circ \psi_{g'}^{-1}(a^1,...,a^{m+n}) = a^i & i = m+1,...,m+n \\ & \forall g, g' \in G. \end{array}\right\} \tag{6.6}$$

Moreover, any supermanifold with such an atlas will be super diffeomorphic to $K(G,A)$.

II. Let $\mathbf{h}$ be the $2^{L-1}(m+n)$-dimensional real Lie algebra derived from $B_L \otimes \mathbf{g}$. Then

$$\mathbf{h} = \mathbf{g}_0 \oplus \mathbf{n} \tag{6.7}$$

where $\mathbf{g}_0$ is the Lie algebra of G and $\mathbf{n}$ is a solvable ideal in $\mathbf{h}$. Let N be the simply-connected Lie group with Lie algebra $\mathbf{n}$; then N is homeomorphic to $\mathbb{R}^{2^{L-1}(m+n)-m}$ and $\exp : \mathbf{n} \to N$ is an analytic diffeomorphism.[11] Now the smooth representation $\pi : G \to (\mathrm{aut}\mathbf{g})_0$ which exists by virtue of the graded Lie group structure of (G,A), (c.f. Eq. 6.1), can be used to define a smooth representation $\alpha : G \to \mathrm{aut}N$, as follows: Define

$$\pi' : G \to \mathrm{aut}\mathbf{h}$$

by

$$\pi'(g)(aX) := a\pi(g)(X) \quad \forall a \in B_L, \; X \in \mathbf{g}_{|a|}. \tag{6.8}$$

then $\pi'(g)(\mathbf{n}) = (\mathbf{n})$ and hence $\pi'' : G \to \mathrm{aut}\mathbf{n}$ can be defined by

$$\pi''(g)(Y) = \pi'(g)Y, \quad \forall Y \in \mathbf{n}. \tag{6.9}$$

Finally $\alpha : G \to \mathrm{aut}N$ is defined by

$$\alpha(g)(\exp Y) := \exp(\pi''(g)(Y)) \quad \forall g \in G, \; Y \in \mathbf{n}. \tag{6.10}$$

Define H to be the semi-direct product of G and N with respect to the representation α, i.e., $H = G \times N$ with group operation

$$(g_1,n_1)(g_2,n_2) := (g_1 g_2, n_1 \alpha(g_1)(n_2)). \tag{6.11}$$

Proposition 6.1 (a) H is a $2^{L-1}(m+n)$- dimensional Lie group with Lie algebra $\mathbf{h}$. (b) H is an (m,n)-dimensional super Lie group with graded Lie module $B_L \otimes \mathbf{g}$.

Indication of proof: (a) is established using the atlas $\{(U_g \times N, \phi_g \times n) | g \in G\}$ on H where $\{(U_g, \phi_g)\}$ is the atlas on G defined by equations (6.3) and η is a global analytic coordinate map on N. ($\mathbf{h}$ emerges as the Lie algebra of H because $\pi|_{Ge} = \mathrm{Ad}_g$.) (b) follows directly from (a) by Theorem 5.5.

III. *Proposition* 6.2: H is superdiffeomorphic to $K(G,A)$. That is, there exists a homeomorphism $\gamma : H \to K(G,A)$ such that both γ and γ^{-1} are superanalytic).

Outline of proof: Recall that ϕ_e is a coordinate map on a neighborhood U_1 of the identity e of G, canonical with respect to the basis $\{X_1,...,X_m\}$ of $\mathbf{g}_0$. Let $\{X_{m+1},...,X_{m+n}\}$ be a basis of $\mathbf{g}_1$, so that (with the notation of the Appendix), $\{\beta_\mu \otimes X_i | i = 1,...,m+n; \mu \in M_L, |\mu|, \mu \neq \Omega\}$ is a basis of $\mathbf{n}$. Suppose $\eta : N + \mathbb{R}^{2^{L-1}(m+n-m)}$ are canonical coordinates with respect to this basis; then the analytic chart $(U_1 \times N, \phi_e \times \eta)$ on the neighborhood $U_1 \times N$ of the identity of H can be used to construct a superanalytic chart $(U_1 \times N, \psi_e)$ by the method of Lemma 5.3. Let

$$V_g := U_g \times N$$

and

$$\psi_g : V_g \to B_L^{m,n} \tag{6.12}$$

with

$$\psi_g(xg, p)) = \psi_g((x,p)(g,e')) := \psi_e((x,p)),$$

where e' denotes the identity element of N. Then the atlas $\{V_g, \psi_g) | g \in G\}$ defines the (unique) superanalytic structure on H with respect to which H is a super Lie group. Also $\psi_g(V_g) = \epsilon^{-1}(\phi_g(U_g))$ and it can be proved that, for all g, g' in G, $\psi_g \circ \psi_{g'} \psi_{g'}^{-1}$ satisfies the conditions (6.6). Hence, $K(G,A)$ is superdiffeomorphic to H. ■

7. CONCLUSION

A mathematically rigorous definition of super Lie group has been given, and several results analogous to those of conventional Lie group theory proved. The problem of classifying super Lie groups over finite-dimensional Grassmann algebras has been reduced to the problem of classifying graded Lie modules. Equipped with a precise global definition of a super Lie group, it should be possible to investigate the physical consequences of their global topology.

APPENDIX: NOTATION

A. Sequences of integers

If p is a positive integer, N_p denotes the set of finite sequences of integers $(n_1,\ldots,n_k)$ with $1\leqslant n_i\leqslant p$ for $i=1,\ldots,k$; M_p denotes the set of sequences of integers $\mu=(\mu_1,\ldots,\mu_k)$ with $1\leqslant\mu_1<\mu_2<\cdots<\mu_k\leqslant p$; Ω denotes the empty sequence in M_p; $M_{p,0}(M_{p,1})$ is the subset of M_p made up of sequences containing an even (odd) number of elements.

B. Basis of the Grassmann algebra

$\{\beta_\mu\,|\,\mu\in M_L\}$ is a basis of B_L (the Grassman algebra over $\mathbb{R}^L$) with $\beta_\Omega=1$ (the unit of B_L)

$$\beta_\mu=1\beta_{(\mu_1)}\beta_{(\mu_2)}\cdots\beta_{(\mu_k)}\quad\forall\mu=(\mu_1,\ldots,\mu_k)\ \text{in}\ M_L;$$

and

$$\beta_{(i)}\beta_{(j)}=-\beta_{(j)}\beta_{(i)}\quad\text{for}\ 1\leqslant i,j\leqslant L.$$

C. Grading

The degree of an element v of a graded vector space, algebra, module etc. is denoted $|v|$, with $|v|=0$ or 1 according as to whether v is even or odd.

When considering (m,n)-dimensional supermanifolds, Lie algebras etc., this grading is put on the set $\{1,\ldots,m+n\}:|i|=0$ if $1\leqslant i\leqslant m$ and $|i|=1$ if $m+1\leqslant i\leqslant m+n$.

A grading is put on M_p by

$$|\mu|=k\quad\text{if}\ \mu\in M_{p,k}\quad(k=0\ \text{or}\ 1).$$

D. Summation convention

Repeated latin indices are summed over $\{1,\ldots,m+n\}$ and repeated greek indices are summed over M_L, unless otherwise indicated.

E. Grassmann algebra combination coefficients

Real numbers $F^\alpha_{\sigma_1\cdots\sigma_k}$ are defined (for $\sigma_1,\ldots,\sigma_k\in M_L$) by

$$\beta_{\sigma_1}\cdots\beta_{\sigma_k}=F^\alpha_{\sigma_1\cdots\sigma_k}\beta_\alpha\,. \tag{A1}$$

Since multiplication in B_L is associative,

$$F^\alpha_{\mu\nu}F^\beta_{\alpha\sigma}=F^\beta_{\mu\nu\sigma}=F^\alpha_{\nu\sigma}F^\beta_{\mu\alpha}\,. \tag{A2}$$

Let $n(\sigma)$ denote the number of sequences in M_L which contain σ as a subsequence, and define $A^{\nu\sigma}_\mu$ (for ν,σ,μ in M_L) by

$$A^{\nu\sigma}_\mu=\frac{+1}{n(\sigma)}\quad\text{if}\ \beta_\nu\beta_\sigma=\beta_\mu$$

$$A^{\nu\sigma}_\mu=\frac{-1}{n(\sigma)}\quad\text{if}\ \beta_\nu\beta_\sigma=-\beta_\mu$$

$$A^{\nu\sigma}_\mu=0\quad\text{otherwise.}$$

Then

$$A^{\nu\sigma}_\mu F^\mu_{\nu\rho}=\delta^\sigma_\rho\,. \tag{A3}$$

F. Homeomorphism of $B_L^{m,n}$ and $\mathbb{R}^{2^{L-1}(m+n)}$

$$\iota:B_L^{m,n}\to\mathbb{R}^{2^{L-1}(m+n)}$$

with

$$\iota\Big(\sum_{\mu\in M_{L,0}}x^{1\mu}\beta_\mu,\ldots,\sum_{\mu\in M_{L,0}}x^{m\mu}\beta_\mu,\sum_{\mu\in M_{L,1}}x^{m+1\,\mu}\beta_\mu,\ldots,\sum_{\mu\in M_{L,1}}x^{m+n\,\mu}\beta_\mu\Big)$$
$$:=(x^{1\Omega},x^{1(1,2)},\ldots,x^{2\Omega},x^{2(1,2)}\ldots,x^{m\Omega},x^{m(1,2)}\ldots,x^{m+1(1)},x^{(m+1(2)},\ldots,x^{m+2(1)},x^{m+2(2)},\ldots,x^{m+n(1)},x^{m+n(2)}\ldots).$$

Components of elements of $\mathbb{R}^{2^{L-1}(m+n)}$ will be labelled

$$(i\mu),\quad i=1,\ldots,m+n,\quad\mu\in M_{L,|i|},$$

and thus, given $x\in\mathbb{R}^{2^{L-1}(m+n)}$,

$$\iota^{-1}(x)=\Big(\sum_{\mu\in M_{L,0}}x^{1\mu}\beta_\mu,\ldots,\sum_{\mu\in M_{L,0}}x^{m\mu}\beta_\mu,\sum_{\mu\in M_{L,1}}x^{m+1\mu}\beta_\mu,\ldots,\sum_{\mu\in M_{L,1}}x^{m+n\,\mu}\beta_\mu\Big).$$

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The Lorentz group in the oscillator realization. III. The group SO(3,1)

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Employing the boson operators of Barut and Böhm, we study the oscillator realization of the Lie algebra of the Lorentz group SO(3,1) in the coordinate representation. The construction yields a direct sum of the principal series of representations (j_0,ρ) belonging to the integral or half-integral class. The decomposition of the representation space into the eigenspaces $L^2_{j_0\rho}$ of irreducible representations leads to a two-variable second order realization of the SO(3,1) algebra acting on $f_{j_0,\rho}\in L^2_{j_0\rho}$. The construction is shown to be highly symmetric. While the elements of the SO(2,1) subalgebra are invariant under the pseudorotation group SO(2,2), those of the full SO(3,1) algebra are invariant under the SO(2)×SO(1,1) subgroup of SO(2,2). We use this intrinsic symmetry in the construction to identify the generalized SO(2,1)⊂SO(3,1) eigenbases with the SO(2,2) harmonics in an SO(2)×SO(1,1) basis, and thereby achieve a significant unification among results which would normally appear disconnected.

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1. INTRODUCTION

In practical applications of the unitary representations of noncompact groups many authors[1-6] have utilized the technique of constructing the generators of the group out of a set of harmonic oscillator creation and annihilation operators satisfying the standard commutation relation $[a_i, a_j^\dagger] = \delta_{ij}$. Holman and Biedenharn[1] proposed a construction of this type for the generators of the three-dimensional Lorentz group SO(2,1). This, however, led only to the discrete class of unitary irreducible representations (UIR's) of the group. A very general construction of this type was given by Barut and Böhm,[2] who proposed an oscillator (or boson) realization for the Lie algebra of the conformal group SO(4,2). The oscillator realization of the conformal algebra and of its various subalgebras have been making their appearance for some time in the past in several investigations, some of a physical and some of a mathematical nature. On the physical side this construction has proved to be an important technical expedient in the recent formulation of the quantum theory of composite objects[7,8] using the SO(4,2) fields in which the Lie algebra of SO(4,2) serve the purpose of defining spin and other quantum numbers. On the mathematical side these investigations, which mostly deal with the simplest SO(2,1) subalgebras of SO(4,2), were partly motivated by their applicability in three related areas:

(1) The noncompact subgroups in this construction appear in especially symmetric forms. This has resulted in application to the explicit construction of noncompact bases leading to the evaluation of matrix elements of operators, Clebsch–Gordan coefficients, etc., of SO(2,1) in continuous noncompact bases.[4,5,9]

(2) In contrast to the canonical Gel'fand[10]–Bargmann[11] realizations, this generally leads to a second order operator realization of the Lie algebra which on exponentiation yields a parametrized continuum of integral transforms. This parametrized continuum, which for SO(2,1) includes, as special cases, Fourier, Hankel, Laplace, Gauss–Weierstrass, Bargmann,[12] and Barut–Girardello[13] transforms, has achieved a significant unification in the theory of integral transforms.[3,4]

(3) This has given better understanding of dynamical groups for quantum systems and partial differential equations.[3,4]

The various investigations belonging to these categories have nontrivial connections with the recent observations on the role of canonical transformations in quantum mechanics and can be regarded as natural consequences of an explicit realization of the SO(2,1) oscillator operators in the coordinate representation. These aspects of the boson realizations of SO(2,1) have been quite extensively treated by Moshinsky,[3] Wolf,[4] Mukunda,[5] and co-workers amongst others.[6] As a consequence of these investigations many important results have been established and the theory has reached a satisfactory stage.

None of these investigations,[3-5] however, attempts to go beyond the three dimensional Lorentz group SO(2,1). The object of the present paper, the third of a series,[9] is to offer a parallel analysis for all UIR's of SO(3,1) belonging to the principal series and to study some typical problems, as classified above, associated with the resulting realization of the SO(3,1) algebra.

A major step towards the stated objective is taken by an explicit transcription of the Barut–Böhm SO(3,1) oscillator operators in the coordinate representation. The choice of the representation space, which is intrinsically different from the one considered recently by Barut and co-workers,[7] was motivated by the fact that the construction possesses a higher symmetry,[14] which manifests itself in this realization. As a consequence of this difference in choice, the SO(3,1) generators **J**, **F** as well as J_2, F_2 are realized as second order differential operators acting on $L^2(R_4)$, in contrast to Ref. 7, in which the compact generators **J** of SO(3) are operators of first order while all the Lorentz boosts **F** are those of second order.

The generators **J**, **F** of the group, in this realization, turn out to be invariant under SO(2)×SO(1,1). Hence SO(2) and SO(1,1) are, of course, external symmetry groups acting on $L^2(R_4)$ and are not the subgroups generated by **J**, **F**. The SO(2)–generator X, having a discrete spectrum $j_0(j_0=0,$

$\pm\frac{1}{2}, \pm 1\ldots$), and the SO(1,1)-generator Y, having a continuous spectrum ρ ($-\infty<\rho<+\infty$), are simply related to the Casimir operators of SO(3,1). Every one-dimensional representation (j_0,ρ) of the "representation generating group" SO(2)×SO(1,1), therefore, yields a UIR of the principal series of SO(3,1). The generators F_1, F_2, and J_3 which constitute the SO(2,1) subalgebra have an even larger symmetry—these are invariant under the four-dimensional pseudorotation group $SO(2,2)\approx SU^{(1)}(1,1)\times SU^{(2)}(1,1)$ (local isomorphism).[15] The representations of SO(2,2) on $L^2(R_4)$ are, however, precisely those carried by the SO(2,2) harmonics, and the Casimir invariant of the SO(2,1) subgroup turns out, as expected, to be a simple function of the only nonvanishing Casimir operator of SO(2,2) [Eq. (4.4)]. Thus the problem of construction of the SO(2,1) basis reduces to that of the "spherical harmonics" for the "spectrum generating group" SO(2,2). However, since the representation generating group, i.e., the symmetry group of the elements of the SO(3,1) algebra, is SO(2)×SO(1,1), a complete orthonormal set of SO(2,2) harmonics in the SO(2)×SO(1,1) basis constitute the eigenbases for the reduction SO(3,1)⊃SO(2,1). This aspect of the problem of SO(3,1) in the oscillator realization closely resembles the Clebsch–Gordan (CG) problem of SO(2,1),[16] in which the structure of the CG series for $D_k^+\times D_k^-$ is fully determined by the properties of SO(2,2) harmonics in the SO(2)×SO(2) basis.[5] Our construction, therefore, achieves a significant unification among results which might otherwise appear disjointed and explains why the CG series of SO(2,1) and the SO(2,1) content of SO(3,1) share the same formal structure.

We now briefly outline the contents of the various sections of the present paper. In Sec. 2 we rewrite the oscillator realization of the Lie algebra of SO(3,1)[2] in the coordinate representation and introduce the symmetry groups, namely, the representation generating group SO(2)×SO(1,1), which is the symmetry group of the SO(3,1) algebra, and the spectrum generating group SO(2,2), which is the symmetry group of the SO(2,1) subalgebra. Section 3 deals with an appropriate parametrization of R_4 and yields a two–variable second order realization of the SO(3,1) algebra acting on $L_1^2(R_2)+L_2^2(R_2)$. In Sec. 4 we deal with the problem of explicit construction of a complete orthonormal set of SO(2,2) harmonics in the SO(2)×SO(1,1) basis and identify them as the generalized eigenbases for the reduction SO(3,1)⊃SO(2,1).

2. OSCILLATOR REALIZATION OF THE SO(3,1) ALGEBRA AND THE SYMMETRY GROUPS

The Lie algebra of SO(3,1) is six-dimensional and is spanned by the elements $J_i, F_i (i=1,2,3)$ satisfying

$$[J_i,J_j]=-[F_i,F_j]=i\epsilon_{ijk}J_k,\qquad [J_i,F_j]=i\epsilon_{ijk}F_k. \tag{2.1}$$

The Lie algebra possesses two independent Casimir invariants C_1, C_2, both of the second degree in the generators

$$C_1=\mathbf{J}^2-\mathbf{F}^2,\quad C_2=\mathbf{J}\cdot\mathbf{F}. \tag{2.2}$$

In a UIR of SO(3,1) the six generators would be represented by Hermitian operators, and C_1, C_2 by real numbers. The UIR's can be classified into two families

(a) *The principal series of* UIR's (j_0,ρ): the values of C_1, C_2 for this class are

$$C_1=-1+j_0^2-\rho^2,\quad C_2=j_0\rho, \tag{2.3}$$

where j_0 is a integer or a half-integer and ρ is a real number in the interval $-\infty<\rho<\infty$.

(b) *The supplementary series of* UIR's $(0,i\sigma)$: for this family $j_0=0$ and ρ becomes pure imaginary, $\rho=i\sigma$, where σ is a real number lying in the interval $0<\sigma<1$. In what follows we shall consider only the principal series of UIR's.

The self-adjoint operators **J**, **F** in the oscillator realization are given by[17]

$$\begin{aligned}
J_1&=\tfrac{1}{2}(a_1^\dagger a_3+a_3^\dagger a_1+a_2^\dagger a_4+a_4^\dagger a_2),\\
J_2&=-\tfrac{i}{2}(a_1^\dagger a_3-a_3^\dagger a_1+a_2^\dagger a_4-a_4^\dagger a_2),\\
J_3&=\tfrac{1}{2}(a_1^\dagger a_1+a_2^\dagger a_2-a_3^\dagger a_3-a_4^\dagger a_4),\\
F_1&=-\tfrac{1}{4}(a_1^{\dagger 2}+a_1^2+a_2^{\dagger 2}+a_2^2-a_3^{\dagger 2}-a_3^2-a_4^{\dagger 2}-a_4^2),\\
F_2&=\tfrac{i}{4}(a_1^{\dagger 2}-a_1^2+a_2^{\dagger 2}-a_2^2+a_3^{\dagger 2}-a_3^2+a_4^{\dagger 2}-a_4^2),\\
F_3&=\tfrac{1}{2}(a_1^\dagger a_3^\dagger+a_1a_3+a_2^\dagger a_4^\dagger+a_2a_4),
\end{aligned} \tag{2.4}$$

where a_m and $a_m^\dagger$ are the familiar harmonic oscillator creation and annihilation operators in the coordinate representation

$$a_m=\frac{i}{\sqrt{2}}\left(x_m+\frac{\partial}{\partial x_m}\right),\qquad a_m^\dagger=-\frac{i}{\sqrt{2}}\left(x_m-\frac{\partial}{\partial x_m}\right),\quad m=1,2,3,4. \tag{2.5}$$

The generators satisfy the commutation relations (2.1) and are Hermitian in $L^2(R_4)$:

$$(f,g)=\int_{R_4} f^*(x)g(x)\,d^4x. \tag{2.6}$$

Symmetry group of the SO(2,1) *subalgebra*: We first show that the generators F_1, F_2, and J_3 of the SO(2,1) subgroup are invariant under the transformation

$$x'=ax, \tag{2.7}$$

which keeps invariant the quadratic form

$$x^2=x_1^2+x_2^2-x_3^2-x_4^2. \tag{2.8}$$

To make the symmetry of these generators explicit we introduce a metric tensor $g_{\mu\nu}$ such that

$$g_{11}=g_{22}=-g_{33}=-g_{44}=1,\qquad \partial_\mu=\partial/\partial x^\mu,\quad x\cdot\partial=x^\mu\partial_\mu,\quad \Box=\partial_\mu\partial^\mu. \tag{2.9}$$

Using Eqs. (2.4), (2.5), and (2.9), the generators F_1, F_2, and J_3 can now be written in the manifestly O(2,2) invariant forms,

$$F_1=\tfrac{1}{4}(x^2+\Box),\quad F_2=\tfrac{i}{2}(x\cdot\partial+2),\quad J_3=\tfrac{1}{4}(x^2-\Box). \tag{2.10}$$

For the purpose of the present paper it is sufficient to consider just the component of O(2,2) containing the identity, namely, SO(2,2). It then follows that the generators

$$M_{\mu\nu} = i(x_\mu \partial_\nu - x_\nu \partial_\mu) \tag{2.11}$$

of SO(2,2) in $L^2(R_4)$ commute with the generators of the SO(2,1) subalgebra:

$$[F_1, M_{\mu\nu}] = [F_2, M_{\mu\nu}] = [J_3, M_{\mu\nu}] = 0. \tag{2.12}$$

The Eq. (2.12), which can be verified by explicit calculation, expresses the symmetry properties of the elements of the SO(2,1) subalgebra, the corresponding symmetry group being SO(2,2).

Symmetry group of the SO(3,1) *algebra*: The generators J_i, F_i, as given by Eqs. (2.4), spanning the SO(3,1) algebra, however, admit of lesser symmetry, the corresponding symmetry group being the SO(2)×SO(1,1) subgroup of SO(2,2). To obtain the transformation induced by this subgroup in R_4 we shall exploit the two-to-one homomorphism of $SU^{(1)}(1,1)\times SU^{(2)}(1,1)$ onto SO(2,2), which states that for every $u^{(i)}\in SU^{(i)}(1,1)$, $i = 1,2$, there is a transformation $a\in SO(2,2)$, with

$$a = T^{-1}(u^{(1)}\times u^{(2)})T, \tag{2.13}$$

where T is a numerical matrix

$$T = \begin{pmatrix} 1 & -i & 0 & 0 \\ 0 & 0 & 1 & i \\ 0 & 0 & 1 & -i \\ 1 & i & 0 & 0 \end{pmatrix}. \tag{2.14}$$

The generators F_3, J_1, and J_2 lying outside the SO(2,1) subalgebra are, of course, not invariant under all transformations of the form

$$x' = T^{-1}(u^{(1)}\times u^{(2)})Tx. \tag{2.15}$$

If however, we restrict ourselves to the SO(2) and SO(1,1) subgroups of $u^{(1)}$ and $u^{(2)}$ so that

$$x' = T^{-1}\left[\begin{pmatrix} e^{i\alpha/2} & 0 \\ 0 & e^{-i\alpha/2} \end{pmatrix} \times \begin{pmatrix} \cosh(\eta/2) & -i\sinh(\eta/2) \\ i\sinh(\eta/2) & \cosh(\eta/2) \end{pmatrix}\right] Tx, \tag{2.16}$$

then all the generators **J**, **F** given by Eq. (2.4) do remain invariant. It now follows that the infinitesimal generators of the transformation (2.16)

$$X = \frac{i}{2}\left(x_1 \frac{\partial}{\partial x_2} - x_2 \frac{\partial}{\partial x_1} + x_3 \frac{\partial}{\partial x_4} - x_4 \frac{\partial}{\partial x_3}\right) = \tfrac{1}{2}(M_{12} - M_{34}) \tag{2.17}$$

and

$$Y = \frac{i}{2}\left(x_1 \frac{\partial}{\partial x_4} + x_4 \frac{\partial}{\partial x_1} - x_2 \frac{\partial}{\partial x_3} - x_3 \frac{\partial}{\partial x_2}\right) = \tfrac{1}{2}(M_{23} - M_{14}), \tag{2.18}$$

which generate the SO(2) subgroup of $u^{(1)}$ and SO(1,1) subgroup of $u^{(2)}$, respectively, commute with all the elements **J**, **F** of the SO(3,1) algebra:

$$[J_i, X] = [F_i, X] = [J_i, Y] = [F_i, Y] = 0. \tag{2.19}$$

Further, since X, Y generate two commuting subgroups,

$$[X, Y] = 0. \tag{2.20}$$

The Eqs. (2.19) and (2.20), which can be verified by direct calculation, imply that X, Y must be related to the Casimir operators of the Lie algebra of SO(3,1). Explicit calculation indeed shows that

$$C_1 = \mathbf{J}^2 - \mathbf{F}^2 = -1 + X^2 - Y^2, \qquad C_2 = \mathbf{J}\cdot\mathbf{F} = XY. \tag{2.21}$$

Since X is an SO(2) generator, having a discrete spectrum $j_0 = 0, \pm 1/2, \pm 1, \cdots$, and Y is an SO(1,1) generator, having a continuous spectrum $-\infty < \rho < \infty$, the present construction yields a direct sum of the principal series of UIR's of SO(3,1). Thus, corresponding to every one-dimensional UIR (j_0, ρ) of the symmetry group SO(2)×SO(1,1), we have a UIR of the principal series of SO(3,1). This Abelian symmetry group, therefore, plays the role of a representation generating group of SO(3,1). The group SO(2,2), which is the symmetry group of the SO(2,1) subalgebra, on the other hand, generates, as shown in Sec. 4, the SO(2,1) content of SO(3,1) via a complete set of SO(2,2) harmonics in an SO(2)×SO(1,1) basis and is, accordingly, called the spectrum-generating group.

3. PARAMETRIZATION OF R_4 AND SECOND ORDER REALIZATION OF THE SO(3,1) ALBEGRA

The representation D of SO(3,1) generated by **J**, **F** of Eq. (2.4) is reducible and is a direct sum of all the UIR's $\mathscr{D}(j_0, \rho)$ belonging to the principal series of representations:

$$D = \sum_{j_0} \oplus \int_{-\infty}^{\infty} d\rho\, \mathscr{D}^{(j_0,\rho)}. \tag{3.1}$$

The first step in effecting the reduction consists of an appropriate parametrization of R_4 which is particularly suited for the decomposition of the representation space into the eigenspaces $L^2_{j_0,\rho}$ of X, Y. To achieve this we express the whole of R_4 as the union of two domains

$$R_4 = D^{(1)} \cup D^{(2)}, \tag{3.2}$$

where $D^{(1)}$ is the "spacelike" domain

$$x_\mu \in D^{(1)}: x^2 = x_1^2 + x_2^2 - x_3^2 - x_4^2 = r^2, \quad 0 < r < \infty, \tag{3.3}$$

and $D^{(2)}$ is the "timelike" domain

$$x_\mu \in D^{(2)}: x^2 = -r^2, \quad 0 < r < \infty. \tag{3.4}$$

We disregard the "light cone"

$$x^2 = 0,$$

as this is a submanifold of lower dimensions.

In $D^{(n)}$, $n = 1,2$, we introduce

$$u^{D^{(1)}} = \frac{1}{r}\begin{pmatrix} x_1 - ix_2 & x_3 - ix_4 \\ x_3 + ix_4 & x_1 + ix_2 \end{pmatrix} \in SU(1,1), \tag{3.5}$$

$$u^{D^{(2)}} = \frac{1}{r}\begin{pmatrix} x_3 - ix_4 & x_1 - ix_2 \\ x_1 - ix_2 & x_3 + ix_4 \end{pmatrix} \in SU(1,1). \tag{3.6}$$

The required parametrization of $R_4 = D^{(1)} \cup D^{(2)}$ now follows as a consequence of that of $u^{D^{(n)}} \in SU(1,1)$. The choice is dictated by the representation generating group

$SO(2)\times SO(1,2)$, which suggests a parametrization of $u^{D^{(n)}}$ of the "mixed basis" type

$$u^{D^{(n)}}=\begin{pmatrix} e^{i\alpha/2} & 0 \\ 0 & e^{-i\alpha/2}\end{pmatrix}\begin{pmatrix}\cosh(\nu/2) & \sinh(\nu/2)\\ \sinh(\nu/2) & \cosh(\nu/2)\end{pmatrix}\times\begin{pmatrix}\cosh(\eta/2) & i\epsilon_n\sinh(\eta/2)\\ -i\epsilon_n\sinh(\eta/2) & \cosh(\eta/2)\end{pmatrix},$$

$$\epsilon_1=-\epsilon_2=1;\quad 0\leqslant\alpha\leqslant 4\pi;\quad -\infty<\nu<\infty;\quad -\infty<\eta<\infty. \tag{3.7}$$

Combining Eqs. (3.5), (3.6), and (3.7), we obtain the elements x_μ in terms of the radial and polar (or hyperbolic) variables

$$x_\mu\in D^{(1)}:\ x_1=r(A+B),\ x_2=r(C-D),\ x_3=r(E-F),\ x_4=-r(G+H), \tag{3.8a}$$

$$x_\mu\in D^{(2)}:\ x_1=r(E+F),\ x_2=r(G-H),\ x_3=r(A-B),\ x_4=-r(C+D), \tag{3.8b}$$

where

$$\begin{pmatrix}A\\B\end{pmatrix}=\begin{pmatrix}\cosh(\nu/2) & \cosh(\eta/2) & \cos(\alpha/2)\\ \sinh(\nu/2) & \sinh(\eta/2) & \sin(\alpha/2)\end{pmatrix};$$
$$\begin{pmatrix}C\\D\end{pmatrix}=\begin{pmatrix}\sinh(\nu/2) & \sinh(\eta/2) & \cos(\alpha/2)\\ \cosh(\nu/2) & \cosh(\eta/2) & \sin(\alpha/2)\end{pmatrix};$$
$$\begin{pmatrix}E\\F\end{pmatrix}=\begin{pmatrix}\sinh(\nu/2) & \cosh(\eta/2) & \cos(\alpha/2)\\ \cosh(\nu/2) & \sinh(\eta/2) & \sin(\alpha/2)\end{pmatrix};$$
$$\begin{pmatrix}G\\H\end{pmatrix}=\begin{pmatrix}\cosh(\eta/2) & \sinh(\eta/2) & \cos(\alpha/2)\\ \sinh(\nu/2) & \cosh(\eta/2) & \sin(\alpha/2)\end{pmatrix}. \tag{3.9}$$

The relation between the derivatives in the Cartesian and polar variables can be obtained after a laborious calculation and is given by

$$\begin{pmatrix}\partial/\partial x_1\\ \partial/\partial x_2\\ \partial/\partial x_3\\ \partial/\partial x_4\end{pmatrix}=\begin{pmatrix}A+B & -E-F & -G+H & -C-D\\ C-D & -G+H & E+F & -A+B\\ -E+F & A-B & -C-D & G-H\\ G+H & -C-D & -A+B & -E-F\end{pmatrix}\times\begin{pmatrix}r(\partial/\partial r)\\ 2(\partial/\partial\nu)\\ 2\,\mathrm{sech}(\partial/\partial\eta)\\ 2\,\mathrm{sech}(\partial/\partial\alpha)\end{pmatrix}$$

for $x_\mu\in D^{(1)}$. (3.10)

For $x_\mu\in D^{(2)}$, the corresponding relation is easily obtained by symmetry.

The Casimir operators X, Y and the Jacobian have the same form in both $D^{(1)}$ and $D^{(2)}$ and explicit calculation yields

$$X=-i(\partial/\partial\alpha),\quad Y=-i(\partial/\partial\eta),$$
$$d^4x=\tfrac{1}{8}r^3\cosh\nu\, d\nu\, d\eta\, d\alpha. \tag{3.11}$$

The representation space now decomposes into two subspaces and the elements $g(x)\in L^2(R_4)$ will, accordingly, be represented by a pair of functions

$$g=\begin{pmatrix}g_1(r,\nu,\eta,\alpha)\\ g_2(r,\nu,\eta,\alpha)\end{pmatrix},$$

which are the elements of a space $L_1^2(D^{(1)})\dot{+}L_2^2(D^{(2)})$. The inner product in $L^2(R_4)$ now becomes

$$(h,g)=\sum_{j=1}^{2}\tfrac{1}{8}\int\int\int\int r^3\,dr\times\cosh\nu\, d\nu\, d\eta\, d\alpha\; h_j^*(r,\nu,\eta,\alpha)g_j(r,\nu,\eta,\alpha). \tag{3.12}$$

Since X, Y have the same form in both $D^{(1)}$ and $D^{(2)}$, to diagonalize X and Y, g_j must be represented by the appropriate Fourier expansions

$$\begin{pmatrix}g_1\\g_2\end{pmatrix}=\frac{1}{\sqrt{2\pi}}\sum_{j_0=-\infty}^{\infty}e^{ij_0\alpha}\int_{-\infty}^{\infty}d\rho\, e^{i\rho\eta}\times\begin{pmatrix}f_1^{\rho,j_0}(r,\nu)\\ f_2^{\rho,j_0}(r,\nu)\end{pmatrix}. \tag{3.13}$$

The summand-integrand, namely the column vector

$$e^{ij_0\alpha}e^{i\rho\eta}\begin{pmatrix}f_1^{\rho,j_0}(r,\nu)\\ f_2^{\rho,j_0}(r,\nu)\end{pmatrix}, \tag{3.14}$$

is by definition the representative element of the eigenspace $L^2_{j_0,\rho}=L^{(2)}_{1;j_0,\rho}\dot{+}L^{(2)}_{2;j_0,\rho}$. The family of these eigenspaces evidently supports the principal series of UIR's of SO(3,1).

Since, in $L^2_{j_0,\rho}$, X and Y can be replaced by the numbers $j_0(j_0=0\pm 1/2,\pm 1\cdots)$ and $\rho(-\infty<\rho<\infty)$, respectively, the above construction yields the desired two-variable second order realization of the SO(3,1) algebra acting on

$$f^{(j_0,\rho)}=\begin{pmatrix}f_1^{j_0,\rho}(r,\nu)\\ f_2^{j_0,\rho}(r,\nu)\end{pmatrix}. \tag{3.15}$$

Acting on the column vector function (3.15), the generators (2.4) will be represented by 2×2 diagonal matrices with operator elements

$$\mathbf{J}=\begin{pmatrix}\mathbf{J}^{(1)} & 0\\ 0 & \mathbf{J}^{(2)}\end{pmatrix},\quad \mathbf{F}=\begin{pmatrix}\mathbf{F}^{(1)} & 0\\ 0 & \mathbf{F}^{(2)}\end{pmatrix}, \tag{3.16}$$

with

$$J_1^{(n)}=\frac{\sinh\nu}{4}\Big[r^2+r\frac{\partial}{\partial r}\Big(\frac{1}{r}\frac{\partial}{\partial r}\Big)-\frac{4\coth\nu}{r}\frac{\partial}{\partial r}\frac{\partial}{\partial\nu}+\frac{8\epsilon_n j_0\rho}{r^2}\mathrm{csch}\nu-\frac{4}{r^2}Q_\nu^{(n)}\Big],$$

$$J_2^{(n)}=\frac{i\epsilon_n}{2}\Big(\sinh\nu r\frac{\partial}{\partial r}-2\cosh\nu\frac{\partial}{\partial\nu}\Big),$$

$$J_3^{(n)}=\frac{\epsilon_n}{4}\Big[r^2-\frac{1}{r^3}\frac{\partial}{\partial r}\Big(r^3\frac{\partial}{\partial r}\Big)-\frac{4}{r^2}Q_\nu^{(n)}\Big],$$

$$F_1^{(n)}=\frac{\epsilon_n}{4}\Big[r^2+\frac{1}{r^3}\frac{\partial}{\partial r}\Big(r^3\frac{\partial}{\partial r}\Big)+\frac{4}{r^2}Q_\nu^{(n)}\Big],$$

$$F_2^{(n)}=\frac{i}{2}\Big(r\frac{\partial}{\partial r}+2\Big),$$

$$F_3^{(n)}=\frac{\sinh\nu}{4}\Big[-r^2+r\frac{\partial}{\partial r}\Big(\frac{1}{r}\frac{\partial}{\partial r}\Big)-\frac{4}{r}\coth\nu\frac{\partial}{\partial r}\cdot\frac{\partial}{\partial\nu}+\frac{8\epsilon_n j_0\rho}{r^2}\mathrm{csch}\nu-\frac{4}{r^2}Q_\nu^{(n)}\Big], \tag{3.17}$$

where

$$Q_\nu^{(n)} = -\frac{1}{\cosh\nu}\left(\frac{\partial}{\partial\nu}\cosh\nu\frac{\partial}{\partial\nu}\right) - \frac{1}{\cosh^2\nu}(j_0^2-\rho^2-2\epsilon_n j_0\rho\sinh\nu),$$

$$\epsilon_1 = -\epsilon_2 = 1.$$

4. THE REDUCTION SO(3,1)⊃SO(2,1) AND SO(2,2) HARMONICS IN SO(2)×SO(1,1) BASIS

We have already seen in Sec. 2 that the generators F_1, F_2, and J_3 of the SO(2,1) subgroup commute with the generators $M_{\mu\nu}$ [Eq. (2.12)] of SO(2,2) acting of $f \in L^2(R_4)$. The representations of SO(2,2) on $L^2(R_4)$, however, belong to a very special type, namely, those for which there is only one nonvanishing Casimir invariant

$$K_1 = -\tfrac{1}{8}M^{\mu\nu}M_{\mu\nu} = -\tfrac{1}{8}M^2. \tag{4.1}$$

The second operator vanishes identically

$$K_2 = \epsilon_{\mu\nu\lambda\sigma}M^{\mu\nu}M^{\lambda\sigma} = 0. \tag{4.2}$$

This has the consequence of restricting the UIR's of SO(2,2) appearing in the problem to the (j,j) type. The commutation relations (2.12), therefore, suggest that the SO(2,1) Casimir invariant

$$Q_{\mathrm{SO}(2,1)} = J_3^2 - F_1^2 - F_2^2 \tag{4.3}$$

must be a function of K_1 and can now be easily verified to essentially coincide with the nontrivial Casimir operator of SO(2,2)

$$Q_{\mathrm{SO}(2,1)} = K_1 = -\tfrac{1}{8}M^2. \tag{4.4}$$

The Eqs. (2.21), in addition, require that in a UIR of SO(3,1), X and Y (and hence C_1 and C_2) must be diagonal. The eigenfunction of $K_1 = -\frac{1}{8}M^2$ will belong to a definite UIR of SO(2,1)⊂SO(3,1); at the same time they will be the basis vectors for the UIR's of SO(2,2) in a definite form, namely, one in which M^2, X and Y are simultaneously diagonal. Since $(X,Y) = \frac{1}{2}(M_{12}-M_{34}, M_{23}-M_{14})$ are the generators of the SO(2)×SO(1,1) subgroup, the representations (j,j) of SO(2,2) appearing in the problem are explicitly reduced under SO(2)×SO(1,1). The eigenbases for the reduction SO(3,1)⊃SO(2,1) which are simultaneous eigenfunctions of

$$-\tfrac{1}{8}M_{\mu\nu}M^{\mu\nu},\ \tfrac{1}{2}(M_{12}-M_{34}),\ \tfrac{1}{2}(M_{23}-M_{14})$$

are, therefore, the SO(2,2) harmonics in SO(2)×SO(1,1) basis.

These SO(2,2) harmonics will evidently involve the angular, or hyperbolic, variables introduced in Sec. 3, leaving the radial dependence unspecified. To completely specify the basis in $L^2_{j_0\rho}$ we need to specify the diagonal generator of SO(2,1)⊂SO(3,1). There are three distinct possibilities; (a) diagonalization of J_3 leading to the reduction SO(3,1)⊃SO(2,1)⊃SO(2), (b) diagonalization of F_2 leading to the reduction SO(3,1)⊃SO(2,1)⊃SO(1,1), and (c) diagonalization of J_3+F_1 leading to SO(3,1)⊃SO(2,1)⊃T_1.

Construction of SO(2,2) *Harmonics*: Having identified the generalized SO(2,1) eigenbases with the SO(2,2) harmonics in SO(2)×SO(1,1) basis, we now deal with its explicit construction. As stated above, these are simultaneous eigenfunctions of

$$Q_{\mathrm{SO}(2,1)} = -\tfrac{1}{8}M^2 = -Q_\nu^{(n)} = \left[\frac{1}{\cosh\nu}\frac{\partial}{\partial\nu}\left(\cosh\nu\frac{\partial}{\partial\nu}\right) + \frac{1}{\cosh^2\nu}\left(\frac{\partial^2}{\partial\eta^2} - \frac{\partial^2}{\partial\alpha^2} - 2\epsilon_n\frac{\partial}{\partial\alpha}\cdot\frac{\partial}{\partial\eta}\sinh\nu\right)\right], \tag{4.5}$$

$$X = -i(\partial/\partial\alpha),\quad Y = -i(\partial/\partial\eta).$$

These are, therefore, of the form

$$y^{(n)}_{j;j_0,\rho}(\alpha,\eta,\nu) = e^{ij_0\alpha}e^{i\rho\eta}f_j^{(n)}(\nu). \tag{4.6}$$

$f_j^{(n)}$ is a solution of the ordinary differential equation

$$-\frac{d}{dz}z(1-z)\frac{df_j^{(n)}}{dz} + \frac{1}{4z(1-z)} \times (j_0^2-\rho^2-2ij_0\rho\epsilon_n(2z-1)) = j(j+1)f_j^{(n)}, \tag{4.7}$$

with

$$z = \tfrac{1}{2}(1-i\sinh\nu),$$

and is given by

$$f_j^{(n)} = z^{(i\rho\epsilon_n+j_0)/2}(1-z)^{(i\rho\epsilon_n-j_0)/2} \times F(-j+i\rho\epsilon_n, j+1+i\rho\epsilon_n; j_0+i\rho\epsilon_n+1; z). \tag{4.8}$$

To ensure the correctness of the choice of solution, we now proceed to show that the family of solutions (4.8) for j running over all continuous nonexceptional representations $j = -\frac{1}{2}+is$, $0<s<\infty$, and a subset of discrete representations, 1(or 3/2)$\leqslant -j \leqslant j_0$, constitute a complete orthogonal set in $L^2_{n;j_0\rho}$.

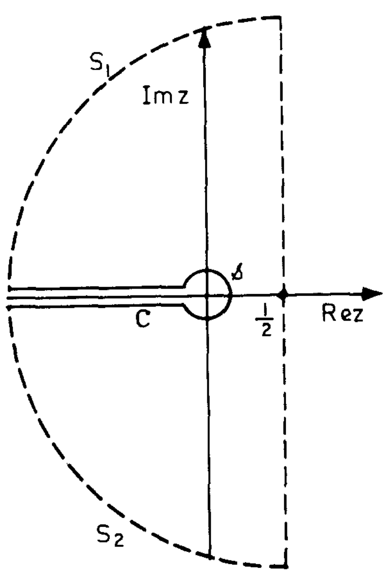

FIG. 1. The contour Σ.

(a) *Orthogonality*: For definiteness, we first consider j lying in the continuous spectrum D^c. The norm of the function $f_j^{(n)} \in L^2_{n;j_0\rho}$ $(n = 1,2)$, is now given by

$$(f_j^{(n)}, f_l^{(n)}) = \int_{-\infty}^{\infty} \cosh\nu \, d\nu \, f_j^{(n)*} f_l^{(n)}. \tag{4.9}$$

On introducing $z = \frac{1}{2}(1 - i\sinh\nu)$, the r.h.s. can be written as a line integral along $\mathrm{Re}z = 1/2$. Setting $n = 1$ and suppressing, for notational convenience, the superscripts we obtain

$$(f_j, f_l) = -2i \int_{1/2 - i\infty}^{1/2 + i\infty} dz \times F(-j - i\rho, j + 1 - i\rho; j_0 - i\rho + 1; 1 - z) \times F(-l + i\rho, l + 1 + i\rho; j_0 + i\rho + 1; z). \tag{4.10}$$

It is clear that for continuous j, f_j can only be δ-function normalizable and the norm (4.10) exists essentially in the sense of generalized function. The main results can, however, be exhibited by constructing a bilinear functional

$$\phi(z) = \int_{-1/2}^{-1/2 + i\infty} dl \, f_l(z) \chi(l) = (1 - z)^{(i\rho - j_0)/2} z^{(i\rho + j_0)/2} \psi(z), \tag{4.11}$$

where

$$\psi(z) = \int \chi(l) \, F(-l + i\rho, l + 1 + i\rho; j_0 + i\rho + 1; z) \, dl \tag{4.12}$$

and $\chi(l)$ is an arbitrary test function. The space of these test functions is chosen such that $\psi(z)$ is analytic in the domain $\mathrm{Re}z \leqslant 1/2$ and vanishes sufficiently rapidly when $|z| \to \infty$ for $\mathrm{Re}z \leqslant 1/2$. We therefore consider

$$(f_j, \phi) = -2i \int_{1/2 - i\infty}^{1/2 + i\infty} dz \, \psi(z) \times F(-j - i\rho, j + 1 - i\rho; j_0 - i\rho + 1; 1 - z). \tag{4.13}$$

Since $\psi(z)$ is analytic, the only singularity of the integrand for $\mathrm{Re}z \leqslant 1/2$ is the branch point of the hypergeometric function (HGF) at $1 - z = 1$, i.e., at $z = 0$. With the standard choice of the cut for the HGF, the integrand is single valued and analytic (for $\mathrm{Re}z \leqslant 1/2$) in the z-plane assumed cut along the negative real axis from 0 to $-\infty$. If we therefore choose, as shown in Fig. 1, a closed contour Σ, by Cauchy's theorem

$$\int_\Sigma \psi(z) \, F(-j - i\rho, j + 1 - i\rho; j_0 - i\rho + 1; 1 - z) \, dz = 0. \tag{4.14}$$

Since $\psi(z)$ vanishes rapidly on S_1, S_2, we have

$$(f_j, \phi) = 2i \int_C \psi(z) \times F(-j - i\rho, j + 1 - i\rho; j_0 - i\rho + 1; 1 - z) \, dz, \tag{4.15}$$

where C stands for the part of Σ formed by the small circle s of radius ϵ around the origin and the branch cut from $-\epsilon$ to $-\infty$.

Using the standard formula,[18]

$$F(a,b;c;1 - z) = \Gamma\begin{bmatrix} c, c - a - b \\ c - a, c - b \end{bmatrix} F(a,b;a + b - c + 1;z) + \Gamma\begin{bmatrix} c, a + b - c \\ a, b \end{bmatrix} z^{c - a - b} F(c - a, c - b; c - a - b + 1; z), \tag{4.16}$$

Eq. (4.15) takes the following form:

$$(f_j, \phi) = 2i\Gamma\begin{bmatrix} j_0 - i\rho + 1, -j_0 - i\rho \\ -j - i\rho, j + 1 - i\rho \end{bmatrix} \int_C dz \, \psi(z) z^{j_0 + i\rho} F_j^{j_0, i\rho}(z) + 2i\Gamma\begin{bmatrix} j_0 - i\rho + 1, j_0 + i\rho \\ j_0 - j, j_0 + j + 1 \end{bmatrix} \int_C dz \, \psi(z) \, F_j^{-i\rho, -j_0}(z), \tag{4.17}$$

where

$$F_j^{j_0, i\rho}(z) = F(j_0 - j, j_0 + j + 1; j_0 + i\rho + 1; z). \tag{4.18}$$

The integrand in the second term on the r.h.s. of Eq. (4.17), which is regular at $z = 0$, is continuous across the branch cut and the integral, therefore, vanishes. The only contribution to the scalar product (f_j, ϕ), therefore, comes from the first term and we have

$$(f_j, \phi) = 2i\Gamma\begin{bmatrix} j_0 - i\rho + 1, -j_0 - i\rho \\ -j - i\rho, j + 1 - i\rho \end{bmatrix} \int \chi(l) I(j,l) \, dl, \tag{4.19}$$

where

$$I(j,l) = \int_C dz \, z^{j_0 + i\rho} F_j^{(j_0, i\rho)}(z) \, F_l^{(i\rho, j_0)}(z) \tag{4.20}$$

$$= \lim_{\epsilon \to 0} \Big[-2i \sin\pi(j_0 + i\rho) \int_{-\epsilon}^{-\infty} dx \, (-x)^{j_0 + i\rho}(1 - x)^{i\rho - j_0} F_j^{i\rho, j_0}(x) F_l^{i\rho, j_0}(x) + \int_s dz \, z^{j_0 + i\rho} \times (1 - z)^{i\rho - j_0} F_j^{i\rho, j_0}(z) \, F_l^{i\rho, j_0}(z) \Big]. \tag{4.21}$$

The integrals appearing in the r.h.s. of the above equation can be evaluated by using the differential equation satisfied by the HGF and we have

$$\int_{-\epsilon}^{-\infty} dx \, (-x)^{j_0 + i\rho}(1 - x)^{i\rho - j_0} F_j^{i\rho, j_0}(x) F_l^{i\rho, j_0}(x) = \lim_{x \to -\infty} \frac{(-x)^{i\rho + j_0 + 1}(1 - x)^{i\rho - j_0 + 1}}{(j + l + 1)(j - l)}$$

$$\times\left[F_l^{i\rho,j_0}\frac{dF_j^{i\rho,j_0}}{dx} - F_j^{i\rho,j_0}\frac{dF_l^{i\rho,j_0}}{dx}\right] + \frac{\epsilon^{i\rho+j_0+1}}{i\rho+j_0+1}, \tag{4.22}$$

$$\int_\lambda dz\, z^{j_0+i\rho}(1-z)^{i\rho-j_0}F_j^{i\rho,j_0}(z)\,F_l^{i\rho,j_0}(z) = 2i\sin\pi(j_0+i\rho)\frac{\epsilon^{i\rho+j_0+1}}{j_0+i\rho+1}. \tag{4.23}$$

Combining Eqs. (4.19) and (4.21)–(4.23), we finally obtain

$$(f_j,\phi) = 4\sin\pi(j_0+i\rho)\int_{-1/2}^{-1/2+i\infty} dl\,\frac{\chi(l)}{(j-l)(j+l+1)}\lim_{x\to-\infty}(-x)^{i\rho+j_0+1}(1-x)^{i\rho-j_0+1}$$

$$\times\left(F_l^{i\rho,j_0}\frac{dF_j^{i\rho,j_0}}{dx} - \frac{dF_l^{i\rho,j_0}}{dx}F_j^{i\rho,j_0}\right). \tag{4.24}$$

Evaluating the r.h.s. in the traditional way we have

$$(f_j,f_l) = 8\pi^2\Gamma\left[\begin{matrix} j_0+i\rho+1,\ j_0-i\rho+1,\ 2j+1,\ -2j-1, \\ -j-i\rho, j+1+i\rho,\ -j+i\rho, j+1-i\rho, j_0-j, j_0+j+1\end{matrix}\right]\delta(\mathrm{Im}\,j-\mathrm{Im}\,l),$$

$$\text{for } \mathrm{Im}\,j,\ \mathrm{Im}\,l>0. \tag{4.25}$$

The orthonormalized SO(2,2) harmonics in $L^{(2)}_{n;j\eta,\rho}$ are, therefore, given by

$$Y^{(n)}_{j;j_0\rho} = N_{j;j_0\rho}e^{ij_0\alpha}e^{i\rho\eta}f_j^{(n)}, \tag{4.26}$$

where

$$N_{j;j_0\rho} = \frac{1}{2\pi^2}\left\{\Gamma\left[\begin{matrix}-j-i\rho, j+1+i\rho,\ -j+i\rho, j+1-i\rho, j_0-j, j_0+j+1, \\ j_0+i\rho+1,\ j_0-i\rho+1,\ 2j+1,\ -2j-1\end{matrix}\right]\right\}^{1/2}. \tag{4.27}$$

Completeness: The completeness of the orthonormalized SO(2,2) harmonics is a direct consequence of that for the SU(1,1) representation functions of Bargmann.[11] The latter have been identified by Mukunda[5] as the SO(2,2) harmonics in an SO(2)×SO(2) basis. The completeness of these SO(2,2) harmonics, therefore, follows from the Plancherel formula for SU(1,1), which states that every square integrable function $f(g)$ on SU(1,1) can be expanded in terms of the representation matrices $D^j_{j_0l}(g)$ as follows:

$$f(g) = \underset{j}{S}\sum_{j_0l}\mu^j_{j_0l}\,D^j_{j_0l}(g). \tag{4.28}$$

Here S stands for the summation over the discrete and integration over the continuous j values. Bargmann's theorem asserts that the UIR's not appearing in the expansion are those of the continuous exceptional series, and the lowest ones ($D^{1/2;\pm}$) of the discrete series.

Analysis of the Plancherel formula[5] for functions $f^{(n)}_{j_0l}$ restricted to the eigenspace $L^{(2)}_{n;j_0l}$, carrying definite SO(2)×SO(2) quantum numbers reveals that only the subset $-1/2>j\geqslant -j_0$ of the discrete UIR's appear in the expansion. The completeness condition can therefore be expressed as

$$f^{(n)}_{j_0l}(g) = -i\int_{-1/2}^{-1/2+i\infty} dj\,\mu(j_0,l;j;n)D^j_{j_0,\epsilon_n l}$$

$$+\sum_{j=-1(\text{or }-3/2)}^{-j_0}\nu(j_0,l;j;n)D^{j;\epsilon_n}_{j_0,\epsilon_n l}, \tag{4.29}$$

where $\epsilon_n=\pm$ according as $n=1$ or 2. Here, for definiteness, we have chosen j_0,l to be positive integers or half-integers and $j_0<l$. If j_0 exceeds l then, of course, the discrete UIR's do not extend beyond $-l$. This equation yields the CG series for the product $D^+\times D^-$.[5]

The above equation, which expresses the completeness of the SO(2,2) harmonics, is a direct consequence of the Plancherel formula for SU(1,1), due to Bargmann.[11] Although the completeness property is established by examining the properties of the SO(2,2) harmonics in the maximal compact SO(2)×SO(2) basis, it is clear that the real content of the result is independent of the basis chosen in setting up the representations of SO(2,2). It is, therefore, possible to transcribe the above result to the situation wherein the SO(2,2) harmonics are constructed in a different basis, namely, in an SO(2)×SO(1,1) basis. Since only a change of basis is involved, the representation functions $D^j_{j_0l}$ of Mukunda will be a linear combination of $Y^{(n)}_{j;j_0\rho}$ given by Eqs. (4.26) and (4.27):

$$D^j_{j_0,\epsilon_n l} = \int_{-\infty}^{\infty} d\rho\, a(j_0,l,\rho;j;n)Y^{(n)}_{j;j_0\rho}. \tag{4.30}$$

The elements $f^{(n)}_{j_0\rho}\in L^2_{n;j_0\rho}$, in addition, can be related to $f^{(n)}_{j_0l}$ of Eq. (4.29) by

$$f^{(n)}_{j_0\rho} = \sum_l a(j_0,\rho,l;n)f^{(n)}_{j_0l}. \tag{4.31}$$

Putting all these facts together, we can easily transcribe the completeness condition (4.28) to read

$$f^{(n)}_{j_0\rho}(g) = -i\int dj\,\lambda(j_0,\rho,j;n)Y^{(n)}_{j;j_0\rho}$$

$$+\sum_{j=-1(\text{or }-3/2)}^{-j_0}\tau(j_0,\rho;j;n)Y^{(n)}_{j;j_0\rho}.$$

In the discrete summation $n=1$ will correspond to the $+ve$ discrete series and $n=2$ to the $-ve$ discrete series, respectively. While the completeness relation expressed in the SO(2)×SO(2) basis yields the structure of the CG series for $D^+\times D^-$, the same relation expressed in the SO(2)×SO(1,1) basis yields the SO(2,1) content of SO(3,1).

The radial eigenfunctions corresponding to the three possible subgroup reductions of $SO(2,1)\subset SO(3,1)$ are as follows:

(i) $SO(3,1)\supset SO(2,1)\supset SO(2)$. In this case J_3 is diagonal and the radial eigenfunctions are given, as in Ref. 9, by Whittaker functions

$$\psi_m^{(n)}(r) = x^{-1} W_{\epsilon_n m, j+1/2}(x),$$
$$x = r^2.$$

(ii) $SO(3,1)\supset SO(2,1)\supset SO(1,1)$. For this subgroup reduction we choose the generator F_2 diagonal. The eigenfunctions are

$$f_\lambda^{(n)}(r) = r^{2i\lambda - 2}.$$

(iii) $SO(3,1)\supset SO(2,1)\supset T_1$. In this case $J_3 + F_1$ is diagonal and the eigenfunctions are

$$g_\mu^{(n)}(r) = \delta(r - |\mu|).$$

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Partial-range completeness and existence of solutions to two-way diffusion equations

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Separating variables to solve a two-way diffusion equation leads to a nonstandard eigenvalue problem in one variable. It is shown that the eigenfunctions having negative eigenvalues are complete on the part of the domain where initial conditions are imposed, while those with positive eigenvalues are complete where final conditions are imposed. The corresponding exponentially growing and exponentially decaying solutions may be used to expand arbitrary solutions on semi-infinite intervals in the "time" variable. A natural iterative procedure for obtaining solutions on finite intervals is shown to converge. In some cases a linearly growing solution must also be taken into account.

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I. INTRODUCTION

We consider the equation

$$h(\theta)\frac{\partial}{\partial x}f(x,\theta)=\frac{\partial}{\partial\theta}D(\theta)\frac{\partial}{\partial\theta}f(x,\theta) \qquad (1)$$

in the domain $a_0<\theta<b_0$ and $0<x<L$, with $D(\theta)$ positive but with $h(\theta)$ changing sign in the interval. Self-adjoint boundary conditions (independent of x) are imposed at $\theta=a_0$ and $\theta=b_0$. Since h changes sign, the usual initial conditions are replaced by initial and final conditions

$$f(0,\theta)=v_+(\theta),\quad \text{where } h(\theta)>0\,, \qquad (2a)$$

$$f(L,\theta)=v_-(\theta),\quad \text{where } h(\theta)<0\,. \qquad (2b)$$

This equation, some physical systems that it describes, and the relevant literature have been discussed by Fisch and Kruskal,[1] so we shall be rather brief here.

The special case

$$\sin\theta\cos\theta\frac{\partial f}{\partial x}=\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}f \qquad (3)$$

for $0<\theta<\pi$, describing the steady-state distribution of particles scattered by a slab, was derived by Bothe.[2] Bethe, Rose, and Smith[3] treated (3) by separation of variables, expanding the solution as a sum of exponential solutions and a single nonexponential or "diffusion solution." Since the eigenvalue problem is not of classical type, however, the question of completeness of the eigenfunctions remained open. The author[4] used methods of functional analysis to prove existence and uniqueness of solutions to (3) and to justify the Bethe–Rose–Smith expansion.

Fisch and Kruskal[1] proved completeness of the eigenfunctions corresponding to the general equation (1) by an extension of classical arguments for the Sturm–Liouville theory, and found conditions for the existence of a diffusion solution. The existence question for (1) was left open, but Fisch and Kruskal pointed out that it was closely related to the conjecture that the eigenfunctions corresponding to negative (respectively positive) eigenvalues are complete in the region where $h(\theta)$ is positive (respectively negative); they also adduced numerical evidence for the conjecture.

In this paper we prove the Fisch–Kruskal conjecture and the existence of solutions to the general problem (1), (2). Similar results were obtained for analogous problems in Ref. 5. However, these results are not immediately applicable to the general equation (1). Moreover, the treatment in Ref. 5 is rather abstract, and for the case of partial differential equations the methods are merely sketched. Therefore we give here a full and self-contained treatment of the problem (1), (2) by adapting some of the methods of Ref. 5. In the process we obtain a different proof of the Fisch–Kruskal completeness theorem, as well as different proofs of the results of Ref. 4.

The paper is organized as follows. In Sec. II we prove completeness of the eigenfunctions associated to the problem by formulating an equivalent self-adjoint problem. Having completeness, we derive the general form of a solution to (1). In Sec. III we prove the partial-range completeness of the eigenfunctions, i.e., the Fisch–Kruskal conjecture. The conjecture is shown to be equivalent to the invertibility of a certain operator built from projections that are self-adjoint with respect to two distinct inner products. The proof of invertibility involves some algebraic manipulations with these projections in order to establish inequalities that imply invertibility.

The partial-range completeness immediately implies the existence of solutions to the problems corresponding to (1), (2), but on the intervals $0<x<\infty$ or $-\infty<x<L$. In Sec. IV we obtain the existence of solutions on finite intervals by reducing the problem to invertibility of still another operator constructed from projections.

These arguments are worked out in detail for the case considered by Fisch and Kruskal, i.e., when there is a diffusion solution. It is pointed out in Sec. II that there are two other cases for Eq. (1). In Sec. V we indicated briefly how these cases may be treated in essentially the same way; in fact they are slightly simpler.

In Sec. VI we consider a natural iterative procedure for constructing solutions on finite intervals, based on the partial-range completeness result. This procedure is shown to converge; in fact it is simply a more concrete version of the operator-theoretic solution given in Sec. IV.

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In Sec. VII we summarize our results for all three cases arising in connection with Eq. (1) and the problem (1), (2).

II. COMPLETENESS OF THE EIGENFUNCTIONS; EXPANSION OF SOLUTIONS

We assume that $D(\theta)$ is such that the standard Sturm–Liouville theory applies to the operator A,

$$Au(\theta) = \frac{d}{d\theta} D(\theta) \frac{d}{d\theta} u(\theta), \tag{4}$$

with the given boundary conditions. Thus there are eigenfunctions φ_k, $k = 0,1,2,\cdots$, and eigenvalues $0 \leqslant \mu_0 \leqslant \mu_1 \leqslant \cdots$ such that

$$A\varphi_k + \mu_k \varphi_k = 0, \tag{5}$$

$$\int \varphi_j(\theta)\varphi_k(\theta)\, d\theta = \delta_{jk}. \tag{6}$$

Three cases should be distinguished:

$$\mu_0 > 0, \tag{7}$$

$$\mu_0 = 0 \text{ and } \int h(\theta)\, d\theta \neq 0, \tag{8}$$

$$\mu_0 = 0 \text{ and } \int h(\theta)\, d\theta = 0. \tag{9}$$

(We assume that h is piecewise continuous, with a piecewise continuous derivative.) All three cases may be treated in essentially the same way. We shall concentrate on the third case, which is slightly more complicated, and discuss the cases (7) and (8) very briefly in Sec. V.

Separating variables in Eq. (1) leads immediately to the following eigenvalue problem:

$$Au_k(\theta) = \lambda_k h(\theta) u_k(\theta). \tag{10}$$

Note that under assumption (9) the equation $Au = v$ has a solution u satisfying the boundary conditions if and only if $\int v(\theta)\, d\theta = 0$. Thus the solutions to (10) must satisfy

$$\int h(\theta) u_k(\theta)\, d\theta = 0 \tag{11}$$

if $\lambda_k \neq 0$. Assumption (9) also implies that there is a function g satisfying the boundary conditions such that

$$Ag = h. \tag{12}$$

Then we must have

$$0 = \int h(\theta) u_k(\theta)\, d\theta = \int Ag(\theta) u_k(\theta)\, d\theta$$
$$= \int g(\theta) A u_k(\theta)\, d\theta = \lambda_k \int g(\theta) h(\theta) u_k(\theta)\, d\theta. \tag{13}$$

Because of (12) and (13), it is natural to look for solutions to (10) in the space H that consists of functions satisfying the boundary conditions and also the two constraints

$$\int h(\theta) u(\theta)\, d\theta = 0 = \int h(\theta) g(\theta) u(\theta)\, d\theta. \tag{14}$$

In this space H we define an inner product

$$\langle u,v \rangle = -\int Au(\theta) v(\theta)\, d\theta = \int D(\theta) \frac{du}{d\theta}\frac{dv}{d\theta}\, d\theta. \tag{15}$$

This inner product is positive definite on H. In fact, suppose $\langle u,u\rangle = 0$; then, since D is positive, it follows from (15) that u is constant. Now

$$0 \neq \int D(\theta)\left(\frac{dh}{d\theta}\right)^2 = -\int g(\theta) h(\theta)\, d\theta. \tag{16}$$

Since u is constant and satisfies (14), we must have $u = 0$.

Suppose v belongs to H. Then there is a unique solution to the problem

$$u \in H, \quad Au = hv. \tag{17}$$

In fact, since v is in H, it satisfies the condition for solvability of $Au = hv$. Let u_0 be a solution. We claim that there is a unique constant α such that $u = u_0 - \alpha$ belongs to H. We must have

$$0 = \int (u_0 - \alpha) h = \int u_0 h = \int u_0 A g = \int (Au_0) g$$
$$= \int hvg, \tag{18}$$

but this is automatic, since v is in H. We must also have

$$0 = \int (u_0 - \alpha) gh = \int u_0 gh - \alpha \int gh. \tag{19}$$

Because of (16), Eq. (19) has a unique solution α.

Let Sv denote the unique solution to (17). Thus S is an operator from H to itself. It is self-adjoint with respect to the inner product (15):

$$\langle Sv_1, v_2\rangle = -\int A(Sv_1) v_2 = -\int hv_1 v_2 = -\int v_1 A(Sv_2)$$
$$= \langle v_1, Sv_2\rangle. \tag{20}$$

Moreover, S is a compact operator in the space H (see Appendix). It follows that H has an orthonormal basis consisting of eigenfunctions for S (see Ref. 6). Note that $Su = 0$ only if $u(\theta) = 0$ where $h \neq 0$. Thus we shall discard the eigenfunctions corresponding to eigenvalue zero. The remaining eigenfunctions u_k satisfy (10) with $\lambda_k \neq 0$. We shall index them so that

$$\lambda_k < 0 \text{ if } k > 0, \quad \lambda_k > 0 \text{ if } k < 0. \tag{21}$$

We may now show that any function u that satisfies the boundary conditions and the conditions

$$\int u^2 < \infty, \quad \int D(\theta)\left(\frac{du}{d\theta}\right)^2 < \infty \tag{22}$$

can be expanded uniquely, where $h(\theta) \neq 0$, in a series

$$u(\theta) = \alpha + \beta g(\theta) + \sum a_k u_k(\theta), \tag{23}$$

where α, β, and the a_k are constants. In fact, by what has already been shown, we only need to show that there are unique constants α and β such that $u - \alpha - \beta g$ belong to H. Thus we need

$$0 = \int (u - \alpha - \beta g) h = \int uh - \beta \int gh, \tag{24}$$

$$0 = \int (u - \alpha - \beta g) h = \int ugh - \alpha \int gh - \beta \int g^2 h. \tag{25}$$

Since $\int gh \neq 0$ by (16), these equations determine α and β uniquely.

Suppose now that f is a solution to (1). We may expand

$$f(x,\theta) = \alpha(x) + \beta(x)g(\theta) + \sum a_k(x)u_k(\theta), \tag{26}$$

where $h(\theta) \neq 0$. From (24) we have

$$\beta(x) = c\int f(x,\theta)h(\theta)\,d\theta, \quad c^{-1} = \int gh, \tag{27}$$

so

$$\frac{d\beta}{dx} = c\int \frac{\partial f}{\partial x}h = c\int Af = 0. \tag{28}$$

Similarly, from (25) we get

$$\alpha(x) = c\int f(x,\theta)g(\theta)h(\theta)\,d\theta - \beta(x)\int g^2 h.$$

Therefore

$$\frac{d\alpha}{dx} = c\int \frac{\partial f}{\partial x}gh = c\int Afg = c\int fAg = c\int fh = \beta. \tag{29}$$

Finally,

$$a_k(x) = \langle f-\alpha-\beta g, u_k\rangle = \int (f-\alpha-\beta g)Au_k$$

$$= \lambda_k\int (f-\alpha-\beta g)hu_k = \lambda_k\int fhu_k, \tag{30}$$

since u_k satisfies (14). Therefore

$$\frac{da_k}{dx} = \lambda_k\int \frac{\partial f}{\partial x}hu_k = \lambda_k\int (Af)u_k = \lambda_k\int fAu_k$$

$$= \lambda_k^2\int fhu_k = \lambda_k a_k.$$

We have shown

$$f(x,\theta) = a + b\,(x + g(\theta)) + \sum a_k e^{\lambda_k x}u_k(\theta), \tag{31}$$

where $h(\theta) \neq 0$. Since the sum on the right gives a solution to (1) that coincides with f wherever $h(\theta) \neq 0$, and since the solution to (1), (2) is unique (see Ref. 1), it follows that (31), is true for all x and θ, $a_0 \leqslant x \leqslant b_0$, $0 \leqslant \theta \leqslant L$.

III. PARTIAL-RANGE COMPLETENESS: THE FISCH-KRUSKAL CONJECTURE

In this section we show that (together with g and a constant function) the eigenfunctions u_k with $\lambda_k < 0$ (respectively, $\lambda_k > 0$) are complete in the region where $h(\theta) > 0$ (respectively, $h(\theta) < 0$). To do this it is convenient to normalize the u_k differently: let

$$v_k = |\lambda_k|^{1/2}u_k. \tag{32}$$

Thus

$$\int hv_jv_k$$

$$= |\lambda_j|^{1/2}|\lambda_k|^{1/2}\int hu_ju_k = |\lambda_j|^{1/2}|\lambda_k|^{1/2}\lambda_j^{-1}\int (Au_j)u_k$$

$$= -|\lambda_j|^{1/2}|\lambda_k|^{1/2}\lambda_j^{-1}\langle u_j,u_k\rangle = -\operatorname{sgn}(\lambda_j)\delta_{jk}. \tag{33}$$

It is also convenient to introduce two new inner products in the space H above:

$$\langle u,v\rangle_1 = \sum \langle u,v_k\rangle\langle v,v_k\rangle, \tag{34}$$

$$\langle u,v\rangle_2 = \int |h(\theta)|u(\theta)v(\theta)\,d\theta. \tag{35}$$

Thus $\langle u,v\rangle_1$ corresponds to taking the v_k as an orthonormal basis in H, while $\langle u,v\rangle_2$ is the L^2 inner product with respect to the measure $|h(\theta)|d\theta$. It is true that the norms associated with these inner products are equivalent: for some constant C,

$$C^{-1}\langle u,u\rangle_1 \leqslant \langle u,u\rangle_2 \leqslant C\langle u,u\rangle_1. \tag{36}$$

However, we shall not need this fact.

We now introduce four projection operators in H. Set

$$P_+u(\theta) = \sum_{k>0}\langle u,v_k\rangle v_k(\theta), \tag{37}$$

$$P_-u(\theta) = \sum_{k<0}\langle u,v_k\rangle v_k(\theta). \tag{38}$$

These are self-adjoint complementary projections with respect to the inner product $\langle u,v\rangle_1$:

$$\langle P_\pm u,v\rangle_1 = \langle u,P_\pm v\rangle_1, \tag{39}$$

$$P_+u + P_-u = u, \tag{40}$$

$$P_+(P_+u) = P_+u, \quad P_-(P_-u) = P_-u. \tag{41}$$

Next, set

$$Q_+u(\theta) = u(\theta), \quad \text{if } h(\theta) > 0,$$
$$Q_+u(\theta) = 0, \quad \text{if } h(\theta) \leqslant 0, \tag{42}$$

$$Q_-u(\theta) = u(\theta), \quad \text{if } h(\theta) \leqslant 0,$$
$$Q_-u(\theta) = 0, \quad \text{if } h(\theta) > 0. \tag{43}$$

Then

$$\langle Q_\pm u,v\rangle_2 = \langle u,Q_\pm v\rangle_2, \tag{44}$$

$$Q_+u + Q_-u = u, \tag{45}$$

$$Q_+(Q_+u) = Q_+u, \quad Q_-(Q_-u) = Q_-u. \tag{46}$$

The following is a basic interrelationship between these four projections and the two inner products:

$$\langle Q_+u - Q_-u,v\rangle_2$$

$$= \int h(\theta)u(\theta)v(\theta)\,d\theta$$

$$= \sum \langle u,v_j\rangle\langle v,v_k\rangle\int h(\theta)v_j(\theta)v_k(\theta)\,d\theta$$

$$= \sum \langle u,v_j\rangle\langle v,v_k\rangle\operatorname{sgn}(j)\delta_{jk} = \langle u,P_+v - P_-v\rangle_1. \tag{47}$$

Since $Q_\pm$ and $P_\pm$ are projections, (47) implies the four basic identities

$$\langle Q_+u,P_+v\rangle_2 = \langle Q_+u,P_+v\rangle_1, \tag{48}$$

$$\langle Q_-u,P_-v\rangle_2 = \langle Q_-u,P_-v\rangle_1, \tag{49}$$

$$\langle Q_+u,P_-v\rangle_2 = -\langle Q_+u,P_-v\rangle_1, \tag{50}$$

$$\langle Q_-u,P_+v\rangle_2 = -\langle Q_-u,P_+v\rangle_1. \tag{51}$$

The partial-range completeness conjecture may be formulated in the following way: if v is in H, then there are unique functions u_+ and u_- in H such that

$$P_+u_+ = u_+ \text{ and } u_+(\theta) = v(\theta), \quad \text{where } h(\theta) > 0, \tag{52a}$$

$$P_-u_- = u_- \text{ and } u_-(\theta) = v(\theta), \quad \text{where } h(\theta) < 0. \tag{52b}$$

In fact, the condition $P_+u_+ = u_+$ is precisely the condition that the expansion of u_+ contains only eigenfunctions with $\lambda_k < 0$, and similarly for the condition $P_-u_- = u_-$. Setting $u = u_+ + u_-$, we may reformulate (52a) and (52b) as the single equation

$$V_1 u = (Q_-P_+ + Q_+P_-)u = v . \tag{53}$$

Our precise statement is that if v belongs to H_2, the completion of H with respect to the inner product (35), Eq. (53) has a unique solution u that belongs to H_1, completion of H with respect to the inner product (34). Note that H_2 consists precisely of functions v such that

$$\int |h(\theta)| v(\theta)^2 \, d\theta < \infty, \quad \int hv = \int ghv = 0 . \tag{54}$$

In proving existence and uniqueness of solutions to (53), it is convenient to introduce three more operators:

$$W_1 = Q_-P_- + Q_+P_+, \quad V_2 = P_+Q_+ + P_-Q_-,$$
$$W_2 = P_+Q_- + P_-Q_+ . \tag{55}$$

Using the properties (39)–(41), (44)–(46), and (48)–(51), one obtains identities

$$\langle V_1u, V_1u\rangle_2 = \langle u,u\rangle_1 + \langle W_1u, W_1u\rangle_2 , \tag{56}$$

$$\langle V_2u, V_2u\rangle_1 = \langle u,u\rangle_2 + \langle W_2u, W_2u\rangle_1 . \tag{57}$$

For example,

$$\begin{aligned}\langle Q_-P_+u, Q_-P_+u\rangle_2 &= \langle Q_-P_+u, P_+u\rangle_2 = \langle Q_-P_+u, P_+u\rangle_1 \\ &= \langle P_+u, P_+u\rangle_1 - \langle Q_-P_+u, P_+u\rangle_1 \\ &= \langle P_+u, P_+u\rangle_1 + \langle Q_-P_+u, P_+u\rangle_2 \\ &= \langle P_+u, P_+u\rangle_1 + \langle Q_-P_+u, Q_-P_+u\rangle_2 .\end{aligned} \tag{58}$$

Interchanging $+$ and $-$ in (58) and adding the new identity to (58) gives (56), and (57) is exactly analogous.

Note that (56) implies $u = 0$ if $V_1u = 0$, so a solution of (53) is unique. It is also an easy consequence of (56) that $V_1(H_1)$ is a closed subspace of the Hilbert space H_2. Therefore, to show that (53) has a solution for every $v \in H_2$, it is enough to show that any element of H_2 orthogonal to all elements V_1u must vanish. But (48) and (50) imply that $\langle v, V_1u\rangle_2 = \langle V_2v, u\rangle_1$. In particular, $\langle v, V_1V_2v\rangle_2 = \langle V_2v, V_2v\rangle_1$. By (57), therefore, if v is orthogonal to all V_1u, it follows that $v = 0$. This shows that (53) has a solution u for each $v \in H_2$.

Another way of expressing the result is this. Suppose only that

$$\int |h(\theta)| v(\theta)^2 \, d\theta < \infty . \tag{59}$$

There are unique constants α, β such that

$$\int (v - \alpha - \beta g)h = 0 = \int (v - \alpha - \beta g)gh . \tag{60}$$

Then $v - \alpha - \beta g$ belongs to H_2, so it may be expanded as above. Thus

$$v(\theta) = \alpha + \beta g(\theta) + \sum_{k>0} a_k v_k(\theta), \quad \text{where } h(\theta) > 0 , \tag{61}$$

and

$$v(\theta) = \alpha + \beta g(\theta) + \sum_{k<0} a_k v_k(\theta), \quad \text{where } h(\theta) < 0 . \tag{62}$$

Note that since the functions v_k are constant multiples of the functions u_k, we may change the constants a_k and replace v_k by u_k in (61) and (62).

For later use we note here some other consequences of the identities (48)–(51), relating the operators V_1 and V_2 and the operators W_1 and W_2:

$$\langle V_1u, v\rangle_2 = \langle u, V_2v\rangle_1, \quad \langle W_1u, v\rangle_2 = -\langle u, W_2v\rangle_1 .$$

Thus if we consider V_1 and W_1 as operators from H_1 to H_2, it follows that the adjoint operators are V_2 and $-W_2$, respectively. Therefore the adjoint of $V_1^{-1} W_1$, considered as an operator in H_1, is $-W_2 V_2^{-1}$. Note finally that if we replace u in the identity (57) by $V_2^{-1}u$, we obtain the inequality

$$\langle W_2V_2^{-1}u, W_2V_2^{-1}u\rangle_1 \leqslant \langle u,u\rangle_1 . \tag{63}$$

IV. EXISTENCE OF SOLUTIONS

Consider first the problem on a semi-infinite interval:

$$h\frac{\partial f}{\partial \theta} = \frac{\partial}{\partial \theta} D(\theta) \frac{\partial f}{\partial \theta}, \quad 0 < x < \infty , \tag{64}$$

$$f(0,\theta) = v(\theta), \quad \text{where } h(\theta) > 0 , \tag{64a}$$

$$f(x,\theta) \to 0 \text{ as } x \to \infty, \quad \text{where } h(\theta) < 0 . \tag{64b}$$

The second condition indicates that the expansion (31) should have only terms for which λ_k is negative. By modifying the function v, where $h(\theta) \leqslant 0$, we may assume that $\int vh = 0 = \int vgh$. Then, by the results of the last section,

$$v(\theta) = \sum_{k>0} a_k u_k(\theta), \quad \text{where } h(\theta) > 0 . \tag{65}$$

Thus with this (unique) choice of the a_k, the solution to (64) is

$$f(x,\theta) = \sum_{k>0} a_k e^{\lambda_k x} u_k(\theta) . \tag{66}$$

Obviously, a similar procedure may be applied to the problem on the interval $-\infty < x \leqslant 0$.

We return now to the original problem (1), (2) on a finite interval $0 \leqslant x \leqslant L$ and seek a solution of the form

$$f(x,\theta) = a + b(x + g(\theta)) + \sum_{k>0} a_k e^{\lambda_k x} u_k(\theta) + \sum_{k<0} a_k e^{\lambda_k (x-L)} u_k(\theta) . \tag{67}$$

To determine the constants a and b we define a function v by

$$v(\theta) = v_+(\theta) - a - bg(\theta), \quad \text{where } h(\theta) > 0 , \tag{68a}$$

$$v(\theta) = v_-(\theta) - a - bL - bg(\theta), \quad \text{where } h(\theta) \leqslant 0 . \tag{68b}$$

If f is to have the form (67) and satisfy the initial and final conditions (2), it follows that Q_+v and Q_-v must belong to Q_+H_1 and Q_-H_1, respectively. Therefore we must have

$$\int h(\theta) v(\theta) \, d\theta = 0 = \int g(\theta) h(\theta) v(\theta) \, d\theta . \tag{69}$$

Equations (68) and (69) determine a and b uniquely.

The preceding argument reduced the problem to that of determining a_k so that the function

$$f^*(x,\theta) = \sum_{k>0} a_k e^{\lambda_k x} u_k(\theta) + \sum_{k<0} a_k e^{\lambda_k (x-L)} u_k(\theta) \tag{70}$$

satisfies the initial and final conditions

$$Q_+f^*(0,\theta) = Q_+v(\theta), \quad Q_-f^*(L,\theta) = Q_-v(\theta), \tag{71}$$

where v belongs to the space H_1 determined by the conditions (69). Define an operator M by

$$Mu_k = e^{-L|\lambda_k|}u_k \tag{72}$$

and define the function u by

$$u(\theta) = \sum a_k u_k(\theta), \tag{73}$$

where the a_k are the same as in (70). Then

$$\begin{aligned} f^*(0,\theta) &= \sum_{k>0} a_k u_k(\theta) + \sum_{k<0} a_k e^{-L\lambda_k} u_k(\theta) \\ &= P_+u(\theta) + P_-Mu(\theta), \end{aligned} \tag{74}$$

where $P_\pm$ are the projections introduced in Sec. III. Similarly,

$$f^*(L,\theta) = P_+Mu(\theta) + P_-u(\theta). \tag{75}$$

Therefore Eqs. (71) may be written

$$\begin{aligned} v &= Q_+(P_+u + P_-Mu) + Q_-(P_+Mu + P_-u) = V_1u + W_1Mu \\ &= V_1(I + V_1^{-1}W_1M)u, \end{aligned} \tag{76}$$

where as before $V_1 = Q_+P_+ + Q_-P_-$ and $W_1 = Q_+P_- + Q_-P_+$.

At this point we have reduced the original problem to the problem of determining the constants a_k in (70), which is equivalent to determining the function u of Eq. (73), which is equivalent to solving (76) for u. Formally, the solution of (76) is given by

$$\begin{aligned} u &= (I + V_1^{-1}W_1M)^{-1}V_1^{-1}v \\ &= \sum_{m=0}^{\infty} (-V_1^{-1}W_1M)^m V_1^{-1}v. \end{aligned} \tag{77}$$

To show that the series (77) converges, it is enough to show that there is a constant $\rho < 1$ such that

$$\langle V_1^{-1}W_1Mu, V_1W_1^{-1}Mu\rangle_1 \leqslant \rho\langle u,u\rangle_1, \tag{78}$$

where $\langle u,v\rangle_1$ is the inner product (34). It is easy to check that

$$\langle Mu,Mu\rangle_1 \leqslant \rho\langle u,u\rangle_1, \tag{79}$$

where ρ is the largest of the numbers $\exp(-2L|\lambda_k|)$, so it is enough to show

$$\langle V_1^{-1}W_1u, V_1^{-1}W_1u\rangle_1 \leqslant \langle u,u\rangle_1. \tag{80}$$

Now (80) is true if and only if the analogous inequality is true for the operator adjoint to $V_1^{-1}W_1$. As remarked at the end of Sec. III, the adjoint operator is $-W_2V_2^{-1}$. The desired inequality for this operator is precisely (63). Therefore the series (77) does converge and determines the solution u. Since u determines the constants a_k in the expansion (70), the original problem is solved (in principle). In Sec. VI we will take another look at the determination of the a_k.

V. OTHER CASES

Our proof of the partial-range completeness and the existence of solutions has been carried out for the case considered by Fisch and Kruskal[1], in which there are "diffusion solutions," i.e., solutions linear in x. This case is characterized by the condition (9). The cases (7) and (8) may be handled in a very similar way; indeed the argument is slightly simpler in these cases. Here we indicated briefly how the preceding arguments should be modified.

In case (7) we may drop the constraints (14) and take H to consist of all functions satisfying the boundary conditions and the condition

$$\int D(\theta)\left(\frac{du}{d\theta}\right)^2 d\theta < \infty.$$

The inner product (15) is positive definite on this space, and the problem (17) has a unique solution $u = Sv$ for every $v \in H$. Again S is a compact self-adjoint operator. Arguing as in Sec. II, we find that any function u in H has an expansion of the form (23), but with $\alpha = \beta = 0$. Therefore a solution to (1) has an expansion (31), with $a = b = 0$. The subsequent discussion carries through also, and we obtain finally the partial-range completeness result of Sec. III and the expansion of Sec. IV, again without a term $a + b[x + g(\theta)]$.

In case (8) we may drop one of the constraints (14) and require in defining H that

$$\int h(\theta)u(\theta)\,d\theta = 0.$$

The inner product (15) is positive definite on H, and the operator S defined above is uniquely determined, compact, and self-adjoint. The arguments above go through once more, giving the expansion (23) with $\beta = 0$, the expansion (31) with $b = 0$, and the expansions in Sec. IV with the constant term a, but without the term $b[x + g(\theta)]$.

VI. CONSTRUCTION OF SOLUTIONS BY ITERATION

Suppose once more that condition (9) is satisfied and that the original problem (1), (2) has been reduced to a problem of the form (1), (70), where v satisfies the conditions (55). In the solution (69) one expects the principal contributions at $x = 0$ to come from the terms with $k > 0$ (so $\lambda_k < 0$), and the principal contributions at $x = L$ to come from the terms with $k < 0$. Therefore a first approximation to the solution would be

$$f_0 = \sum_{k>0} a_{k,0}e^{\lambda_k x}u_k + \sum_{k<0} a_{k,0}e^{\lambda_k(x-L)}u_k,$$

where the constants are chosen so that

$$v(\theta) = \sum_{k>0} a_{k,0}u_k(\theta), \quad \text{if } h(\theta) > 0, \tag{81a}$$

$$v(\theta) = \sum_{k<0} a_{k,0}u_k(\theta), \quad \text{if } h(\theta) < 0. \tag{81b}$$

Then f_0 will satisfy Eq. (1), but we have

$$f_0(0,\theta) = v(\theta) - \sum_{k<0} e^{-\lambda_k L}a_{k,0}u_k(\theta), \quad \text{if } h(\theta) > 0, \tag{82a}$$

$$f_0(L,\theta) = v(\theta) - \sum_{k>0} e^{\lambda_k L}a_{k,0}u_k(\theta), \quad \text{if } h(\theta) < 0. \tag{82b}$$

Thus we want to add a correction term f_1 of the same form as f_0, but with coefficients $a_{k,1}$ determined by

$$-\sum_{k<0} e^{-\lambda_k L}a_{k,0}u_k = \sum_{k>0} a_{k,1}u_k, \quad \text{where } h(\theta) > 0,$$

$$-\sum_{k>0} e^{\lambda_k L}a_{k,0}u_k = \sum_{k<0} a_{k,1}u_k, \quad \text{where } h(\theta) < 0.$$

Continuing in this manner, we construct f of the form (70), where the coefficients a_k are given by series:

$$a_k = \sum_{m=0}^{\infty} a_{k,m} . \tag{83}$$

The initial terms $a_{k,0}$ are given by (80), and succeeding terms are determined iteratively by

$$- \sum_{k<0} e^{-\lambda_k L} a_{k,m} u_k = \sum_{k>0} a_{k,m+1} u_k, \quad \text{where } h(\theta) > 0 , \tag{84a}$$

$$- \sum_{k>0} e^{\lambda_k L} a_{k,m} u_k = \sum_{k<0} a_{k,m+1} u_k, \quad \text{where } h(\theta) < 0 . \tag{84b}$$

This iterative procedure converges; in fact it corresponds precisely to the solution (77). If we set

$$u^{(m)} = \sum_k a_{k,m} u_k , \tag{85}$$

then (81) and (84) become

$$V_1 u^{(0)} = v, \quad V_1 u^{(m+1)} = - W_1 M u^{(m)} , \tag{86}$$

so

$$u^{(m)} = (-V_1^{-1} W_1 M)^m / v \tag{87}$$

and therefore

$$\sum_k a_k u_k = \sum_m u^{(m)} \tag{88}$$

is given by the series in Eq. (77).

In conclusion, we take note of the fact that although equations like (81) and (84) determine the coefficients $a_{k,m}$ implicitly, it is not easy to determine them explicitly. The reason for this is that the eigenfunctions u_k are no longer orthogonal when restricted to the regions where $h(\theta)$ is positive or negative, so one cannot recover the coefficients simply by integrating the known function against the u_k. The coefficients can be approximated by choosing a least-squares approximation with respect to the inner product (35), however. In fact if

$$\sum_{k>0} a_k u_k(\theta) = v(\theta), \quad \text{where } h(\theta) > 0 ,$$

then

$$\int_{h(\theta)>0} h(\theta) \Big[\sum_0^N a_k u_k(\theta) - v(\theta) \Big]^2 d\theta \tag{89}$$

converges to zero as $N \to \infty$, and similarly for the expansion where $h(\theta)$ is negative.

VII. SUMMARY

In order to solve the problem (1), (2), we investigated the operator A,

$$Au(\theta) = \frac{d}{d\theta} D(\theta) \frac{du}{d\theta} , \tag{90}$$

when u satisfies the boundary conditions at $\theta = a_0, b_0$.

Suppose first that 0 is not an eigenvalue of the operator A. Let u_k be the eigenfunctions for the eigenvalue problem

$$Au_k(\theta) = \lambda_k u_k(\theta), \quad \lambda_k \neq 0 , \tag{91}$$

and number the λ_k so that k and λ_k have opposite sign. In the problem (1), (2), define $v(\theta) = v_+(\theta)$, where $h(\theta) > 0$, and $v(\theta) = v_-(\theta)$, where $h(\theta) < 0$; we may take $v(\theta) = 0$, where $h(\theta) = 0$. Then the unique solution to (1), (2) has an expansion

$$f(x,\theta) = \sum_{k>0} a_k e^{\lambda_k x} u_k(\theta) + \sum_{k<0} a_k e^{\lambda_k (x-L)} u_k(\theta) , \tag{92}$$

where the constants a_k are given by convergent series $\Sigma a_{k,m}$, and the $a_{k,m}$ are determined implicitly by Eqs. (81) and (84).

Suppose next that 0 is an eigenvalue of A, i.e., that the constant functions satisfy the boundary conditions, but suppose also that

$$\int h(\theta)\, d\theta \neq 0 . \tag{93}$$

In the problem (1), (2), define

$$\begin{aligned} v(\theta) &= v_+(\theta) - a, \quad \text{if } h(\theta) > 0 , \\ v(\theta) &= v_-(\theta) - a, \quad \text{if } h(\theta) < 0 , \\ v(\theta) &= 0, \quad \text{if } h(\theta) = 0 , \end{aligned} \tag{94}$$

where the constant a is chosen so that

$$\int v(\theta) h(\theta)\, d\theta = 0 . \tag{95}$$

Then the unique solution to (1), (2) has an expansion

$$f(x,\theta) = a + \sum_{k>0} a_k e^{\lambda_k x} u_k(\theta) + \sum_{k<0} a_k e^{\lambda_k (x-L)} u_k(\theta) , \tag{96}$$

where again $a = \Sigma a_{k,m}$ and the $a_{k,m}$ are determined by (81) and (84).

Finally, suppose that 0 is an eigenvalue of A, and that $\int h(\theta)\, d\theta = 0$. Then let g be a solution of $Ag = h$. In the problem (1), (2) define

$$\begin{aligned} v(\theta) &= v_+(\theta) - a - bg(\theta), \quad \text{if } h(\theta) > 0 , \\ v(\theta) &= v_-(\theta) - a - b[L + g(\theta)], \quad \text{if } h(\theta) < 0 , \\ v(\theta) &= 0, \quad \text{if } h(\theta) = 0 , \end{aligned} \tag{97}$$

where the constants a and b are chosen so that

$$\int v(\theta) h(\theta)\, d\theta = 0 = \int v(\theta) g(\theta) h(\theta)\, d\theta . \tag{98}$$

Then the unique solution to (1), (2) has the expansion

$$f(x,\theta) = a + b[x + g(\theta)] + \sum_{k>0} a_k e^{\lambda_k x} u_k(\theta) + \sum_{k<0} a_k e^{\lambda_k (x-L)} u_k(\theta) , \tag{99}$$

where again $a = \Sigma a_{k,m}$ and the $a_{k,m}$ are determined by (81) and (84).

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APPENDIX: COMPACTNESS OF THE OPERATOR S

To show that S is compact we write it as the composition of three operators, show that these operators are continuous with respect to suitably chosen norms, and show that one of the three is compact. For this purpose let

$$Ju(\theta) = h(\theta)u(\theta),$$

$$Bu(\theta) = \sum_{k=1}^{\infty}\left(\int u\varphi_k\right)\mu_k^{-1}\varphi_k,$$

$$Ku(\theta) = u(\theta) - c^{-1}\int ugh,$$

where $c = \int g(\theta)h(\theta)\,d\theta$. Then S is the composition KBJ.

The operator K is continuous from the space of functions u that satisfy the boundary conditions and the conditions

$$\int u(\theta)\,d\theta = 0, \quad \langle u,u\rangle < \infty \tag{A1}$$

to the space H with the inner product $\langle u,v\rangle$. In fact $\langle Ku,Ku\rangle = \langle u,u\rangle$.

The operator B is compact from the space L^2 of functions with inner product $\int uv$ to the space described by (A1). In fact, let $\psi_k = \mu_k^{-1/2}\varphi_k$ for $k \geqslant 1$. Then the φ_k are an orthonormal basis for L^2, the ψ_k are an orthonormal basis for the space (A1), and $B\varphi_k = \mu_k^{-1/2}\varphi_k$. Since $\mu_k \to \infty$ as $k \to \infty$, it follows that B is compact.

The operator J is continuous from H with inner product $\langle u,v\rangle$ to L^2. To see this, write u belonging to H in terms of the orthonormal basis $\{\varphi_k\}$ in L^2:

$$u = c_0\varphi_0 + \sum_{k=1}^{\infty} c_k\varphi_k = c_0\varphi_0 + u_1.$$

Then

$$\int (hu)^2 \leqslant C\int u^2 = C\left(c_0^2 + \int u_1^2\right). \tag{A2}$$

With ψ_k as above,

$$\int u_1^2 = \sum_{k=1}^{\infty} c_k^2 = \sum_{k=1}^{\infty}\left(\int u\varphi_k\right)^2 = \sum u_k\left(\int u\psi_k\right)^2$$
$$= \sum \mu_k^{-1}\left(\int uA\psi_k\right)^2 = \sum \mu_k^{-1}\langle u,\psi_k\rangle^2$$
$$\leqslant \mu_1^{-1}\sum\langle u,\psi_k\rangle^2 \leqslant \mu_1^{-1}\langle u,u\rangle, \tag{A3}$$

since the ψ_k are orthonormal with respect to the inner product $\langle u,v\rangle$. Finally, since we are assuming that u is in H, we have

$$0 = \int ugh = \int c_0\varphi_0 gh - \int u_1 gh,$$

so

$$c_0^2 = \left(\int \varphi_0 gh\right)^{-2}\left(\int u_1 gh\right)^2 \leqslant C_1\int u_1^2 \leqslant C_1\mu_1^{-1}\langle u,u\rangle. \tag{A4}$$

Combining (A2), (A3), and (A4) we get the asserted continuity property of J. In fact, the operator J is also compact, but we do not need this fact.

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Bäcklund transformations for the Ernst equation

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Presented is a systematic approach to the transformation theories for the Ernst equation from the viewpoint of the Bäcklund transformation. It is explicitly shown that the method of Clairin gives a simple derivation of various transformations such as transformations found by Ehlers, Neugebauer, and Harrison.

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1. INTRODUCTION

The Ernst equation deals with the stationary axially symmetric gravitational field. As is well-known there have been found many solutions.[1] Some people[2] have shown that the Ernst equation has remarkable internal symmetries and by using these symmetries have obtained the technique for generating new exact solutions.

In recent years, the methods developed in the theory of solitons have been applied to the Ernst equation. Belinsky–Zakharov,[3] Maison,[4] and Hauser–Ernst[5] have shown that the Ernst equation can be solved by the inverse scattering method. Harrison[6] and Neugebauer[7] have found Bäcklund transformations for the Ernst equation. In particular, Neugebauer has discussed a method to construct various solutions by using the Bäcklund transformation.

The aim of this paper is the presentation of a systematic method to find the transformations for the Ernst equation. Employing the method of Clairin,[8] we shall explicitly show that the Ernst equation has Bäcklund transformations. The outline of the paper is the following. In Sec. 2, we shall formulate the Bäcklund transformation for the Ernst equation, and as a first nontrivial example, derive the transformation given by Ehlers. In Sec. 3, we shall obtain three kinds of Bäcklund transformations. Introducing a pseudopotential for each Bäcklund transformation, these transformations will be found to be equivalent to those of Neugebauer and Harrison in Sec. 4. The last section is devoted to conclusion and discussions.

2. THE ERNST EQUATION AND THE EHLERS TRANSFORMATION

The Ernst equation is written in terms of the Ernst potential E as

$$\partial_\xi\partial_\eta E = -(1/4\rho)(\partial_\xi E + \partial_\eta E) + (1/T)\partial_\xi E\partial_\eta E, \quad (2.1)$$

where $2\rho = \xi + \eta$, $\bar{\xi} = \eta$, and $2T = E + \bar{E}$.

In general, the Bäcklund transformation for a second-order partial differential equation in two independent variables is a pair of first-order partial differential equations which relate a solution to the other solution. Following Clairin, we consider the two Ernst potentials, E and E', related by

$$\partial_\xi E' = P(\partial_\xi E, \partial_\eta E, E, E', \text{c.c.}, \xi, \eta),$$
$$\partial_\eta E' = Q(\partial_\xi E, \partial_\eta E, E, E', \text{c.c.}, \xi, \eta), \quad (2.2)$$

where c.c. denotes the complex conjugates of $\partial_\xi E$, $\partial_\eta E$, E, and E'. We note that apart from the independent variable transformation, Eqs. (2.2) are the most general form of the Bäcklund transformation for the Ernst equation. The functional forms of P and Q are determined from the requirements:

(1) E' satisfies the integrability condition $\partial_\xi\partial_\eta E' = \partial_\eta\partial_\xi E'$,

(2) E' is a solution of the Ernst equation.

In the following we focus our interest on particular forms of P and Q such that

$$P = a_1\partial_\xi E + a_2,$$
$$Q = b_1\partial_\eta E + b_2, \quad (2.3)$$

where a_i and b_i $(i = 1,2)$ are functions of $E, \bar{E}, E', \bar{E}', \xi$, and η. In spite of this simplification we shall find that all the interesting transformations are derived systematically from Eqs. (2.2) with Eqs. (2.3).

The integrability condition for E' gives the following differential equations

$$\nabla_2 a_1 - \nabla_1 b_1 + (1/T)(a_1 - b_1) = 0,$$
$$\bar{\nabla}_1 a_1 = 0, \quad \bar{\nabla}_2 b_1 = 0,$$
$$\partial_\eta a_1 - \nabla_1 b_2 + \bar{\nabla}_3 a_1 - (1/4\rho)(a_1 - b_1) = 0,$$
$$\partial_\xi b_1 - \nabla_2 a_2 + \nabla_3 b_1 + (1/4\rho)(a_1 - b_1) = 0. \quad (2.4)$$

Here, ∇_i and $\bar{\nabla}_i$ $(i = 1,2,3)$ are defined by

$$\nabla_1 = \partial_E + a_1\partial_{E'}, \quad \bar{\nabla}_1 = \partial_{\bar{E}} + \bar{a}_1\partial_{\bar{E}'},$$
$$\nabla_2 = \partial_E + b_1\partial_{E'}, \quad \bar{\nabla}_2 = \partial_{\bar{E}} + \bar{b}_1\partial_{\bar{E}'}, \quad (2.5)$$
$$\nabla_3 = a_2\partial_{E'} + \bar{b}_2\partial_{\bar{E}'}, \quad \bar{\nabla}_3 = \bar{a}_2\partial_{\bar{E}'} + b_2\partial_{E'}.$$

From the requirment of (2) we have

$$\nabla_2 a_1 + (1/T)a_1 - (1/T')a_1 b_1 = 0, \quad (2.6)$$
$$\bar{\nabla}_1 a_1 = 0, \quad (2.7)$$
$$\partial_\eta a_1 + \bar{\nabla}_3 a_1 - (1/T')a_1 b_2 = 0, \quad (2.8)$$
$$\nabla_2 a_2 - (1/4\rho)(a_1 - b_1) - (1/T')b_1 a_2 = 0, \quad (2.9)$$
$$\bar{\nabla}_1 a_2 = 0, \quad (2.10)$$
$$\partial_\eta a_2 + \nabla_3 a_2 + (1/4\rho)(a_2 + b_2) - (1/T')a_2 b_2 = 0, \quad (2.11)$$

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and

$$\nabla_1 b_1 + (1/T)b_1 - (1/T')a_1 b_1 = 0, \tag{2.12}$$

$$\bar{\nabla}_2 b_1 = 0, \tag{2.13}$$

$$\partial_\xi b_1 + \nabla_3 b_1 - (1/T')b_1 a_2 = 0, \tag{2.14}$$

$$\nabla_1 b_2 + (1/4\rho)(a_1 - b_1) - (1/T')a_1 b_2 = 0, \tag{2.15}$$

$$\bar{\nabla}_2 b_2 = 0, \tag{2.16}$$

$$\partial_\xi b_2 + \nabla_3 b_2 + (1/4\rho)(a_2 + b_2) - (1/T')a_2 b_2 = 0, \tag{2.17}$$

where $2T' = E' + \bar{E}'$. Since Eqs. (2.4) are obtained from (2.6)–(2.17), the independent equations which should be considered are (2.6)–(2.17).

At first we shall consider Eqs. (2.6), (2.7), (2.12), and (2.13) which determine the functional forms of a_1 and b_1. By factorizing a_1 and b_1 as

$$a_1 = (T'/T)f, \quad b_1 = (T'/T)g, \tag{2.18}$$

we rewrite Eqs. (2.6), (2.7), (2.12), and (2.13);

$$\partial_E f + (T'/T)g\partial_{E'} f = (f/2T)(g-1), \tag{2.19}$$

$$\partial_{\bar{E}} f + (T'/T)\bar{f}\partial_{\bar{E}'} f = (f/2T)(1-\bar{f}), \tag{2.20}$$

$$\partial_E g + (T'/T)f\partial_{E'} g = (g/2T)(f-1), \tag{2.21}$$

$$\partial_{\bar{E}} g + (T'/T)\bar{g}\partial_{\bar{E}'} g = (g/2T)(1-\bar{g}). \tag{2.22}$$

It is seen that the simplest solution of Eqs. (2.19)–(2.22) is $f = g = 1$. In this case, we have

$$a_1 = b_1 = T'/T, a_2 = b_2 = 0. \tag{2.23}$$

The integration of Eq. (2.2) with Eqs. (2.3) and (2.23) yields

$$E' = CE + iD, \tag{2.24}$$

where C and D are real constants. This transformation is rather trivial.

Next we find a simple but nontrivial solution of Eqs. (2.19)–(2.22);

$$f = g = -(\bar{E} - im)/(E + im), \tag{2.25}$$

wher m is a real constant. The solution (2.25) gives

$$a_1 = b_1 = -\frac{T'}{T}\frac{\bar{E} - im}{E + im},$$
$$a_2 = b_2 = 0, \tag{2.26}$$

and then

$$\partial_\xi E' = -\frac{T'}{T}\frac{\bar{E} - im}{E + im}\partial_\xi E,$$
$$\partial_\eta E' = -\frac{T'}{T}\frac{\bar{E} - im}{E + im}\partial_\eta E. \tag{2.27}$$

By integrating Eq. (2.27), we have

$$E' = (E + ic)/(i\gamma E + d), \tag{2.28}$$

where c, d, and γ are constants. This is equivalent to Ehler's transformation which is extensively used by Kinnersley.

3. BÄCKLUND TRANSFORMATIONS FOR THE ERNST EQUATION

In the preceding section we obtained two simple solutions (2.23) and (2.26). In order to obtain more general solutions we introduce a function γ which satisfies the differential equations

$$\partial_E \gamma = \partial_{\bar{E}} \gamma = \alpha/T,$$
$$\partial_{E'} \gamma = \partial_{\bar{E}'} \gamma = \alpha/T'. \tag{3.1}$$

Here $\alpha = \alpha(\gamma)$ is a function of γ. We assume that f and g depend on γ, ξ, and η only, and do not have the explicit dependence of E, $\bar{E}$, E', $\partial_{\bar{E}}$, and $\bar{E}$. Under the assumption we have

$$\partial_E f = \partial_{\bar{E}} f = (\alpha/T)\dot{f}, \quad \partial_E g = \partial_{\bar{E}} g = (\alpha/T)\dot{g},$$
$$\partial_{E'} f = \partial_{\bar{E}'} f = (\alpha/T')\dot{f}, \quad \partial_{E'} g = \partial_{\bar{E}'} g = (\alpha/T')\dot{g}, \tag{3.2}$$

where $\dot{f} = \partial_\gamma f$ and $\dot{g} = \partial_\gamma g$. By using Eqs. (3.2) we rewrite Eqs. (2.19)–(2.22) as

$$\dot{f} = \frac{f}{2\alpha}\frac{g-1}{g+1}, \tag{3.3}$$

$$\dot{g} = \frac{g}{2\alpha}\frac{f-1}{f+1}, \tag{3.4}$$

$$g\bar{f} = 1. \tag{3.5}$$

We further assume that a_2 and b_2 can be factorized in the form

$$a_2 = T'u(\gamma,\xi,\eta),$$
$$b_2 = T'v(\gamma,\xi,\eta). \tag{3.6}$$

Then equations (2.8)–(2.11) and (2.14)–(2.17) are reduced to

$$\partial_\eta f = f(f-g)/\rho(f+1)(g+1),$$
$$\partial_\xi f = (f-g)(fg+1)/2\rho(g+1)^2 \tag{3.7}$$

$$\partial_\xi g = g(g-f)/\rho(f+1)(g+1),$$
$$\partial_\eta g = (g-f)(fg+1)/2\rho(f+1)^2, \tag{3.8}$$

and

$$u = \frac{1}{2\rho}\frac{g-f}{g+1}, \quad v = \frac{1}{2\rho}\frac{f-g}{f+1}. \tag{3.9}$$

By integrating Eqs. (3.1) we obtain

$$\int d\gamma/2\alpha \equiv \log\theta, \tag{3.10}$$

where θ is defined by

$$\theta = \theta_0 TT'. \tag{3.11}$$

In Eqs. (3.11) θ_0 is a function of ξ, η only.

In the following we will obtain three kinds of Bäcklund transformations.

(i) $f = g$: From Eqs. (3.3)–(3.5) we have

$$\dot{f} = \frac{f}{2\alpha}\frac{f-1}{f+1}, \tag{3.12}$$

$$f\bar{f} = 1. \tag{3.13}$$

This can be easily integrated and $f(=g)$ is given in terms of θ by

$$f = g = [2 + \theta \pm (\theta^2 + 4\theta)^{1/2}]/2. \tag{3.14}$$

Equations (3.7)–(3.9) give

$$u = v = 0, \quad \theta_0 \equiv C = \text{const}. \tag{3.15}$$

Thus we obtain the first Bäcklund transformation

$$\partial_\xi E' = \frac{T'}{T}\frac{2 + \theta \pm (\theta^2 + 4\theta)^{1/2}}{2}\partial_\xi E,$$
$$\partial_\eta E' = \frac{T'}{T}\frac{2 + \theta \pm (\theta^2 + 4\theta)^{1/2}}{2}\partial_\eta E, \tag{3.16}$$

where $\theta = CTT'$.

(ii) $f = 1/g$: Equations (3.3)–(3.5) are reduced to

$$\dot{f} = \frac{f}{2\alpha}\frac{1-f}{f+1}, \tag{3.17}$$

$$f = \bar{f}. \tag{3.18}$$

Integration of Eq. (3.17) yields

$$f = [2\theta + 1 + (4\theta + 1)^{1/2}]/2\theta,$$
$$g = [2\theta + 1 - (4\theta + 1)^{1/2}]/2\theta. \tag{3.19}$$

Equations (3.7) and (3.8) imply that

$$\partial_\xi \log\theta = -1/\rho, \quad \partial_\eta \log\theta = -1/\rho. \tag{3.20}$$

From Eqs. (3.20), θ is given by

$$\theta = (c/\rho^2)TT', \tag{3.21}$$

where c is a constant. By substituting Eqs. (3.19) into Eqs. (3.9), u and v are expressed as

$$u = -[(4\theta + 1)^{1/2} + 1]/4\rho\theta,$$
$$v = [(4\theta + 1)^{1/2} - 1]/4\rho\theta. \tag{3.22}$$

The second Bäcklund transformation for the Ernst equation has therefore the following form:

$$\partial_\xi E' = \frac{T'}{T}\frac{2\theta + 1 + (4\theta + 1)^{1/2}}{2\theta}\partial_\xi E - \frac{T'}{4\rho}\frac{1 + (4\theta + 1)^{1/2}}{\theta},$$
$$\partial_\eta E' = \frac{T'}{T}\frac{2\theta + 1 - (4\theta + 1)^{1/2}}{2\theta}\partial_\eta E - \frac{T'}{4\rho}\frac{1 - (4\theta + 1)^{1/2}}{\theta}, \tag{3.23}$$

where θ is given by (3.21).

(iii) $f = 1/\bar{g}$: By integrating Eqs. (3.3) and (3.4) we find that

$$f = ((k+1)(\theta^2 + 1) - 2k\theta \pm (k+1)(\theta - 1)\{\theta^2 - 2[(k-1)/(k+1)]\theta + 1\}^{1/2})/2\theta,$$
$$g = (-(k+1)(\theta^2 + 1) - 2\theta \mp (k+1)(\theta + 1)\{\theta^2 - 2[(k-1)/(k+1)]\theta + 1\}^{1/2})/2k\theta, \tag{3.24}$$

where $\bar{\theta} = -\theta$, $\bar{k} = 1/k$. Substitution of Eqs. (3.24) into Eqs. (3.7) and (3.8) leads to

$$\theta_\xi = -(1/2\rho)\theta, \quad \theta_\eta = -(1/2\rho)\theta, \tag{3.25}$$

$$k_\xi = -k(k+1)/2\rho, \quad k_\eta = (k+1)/2\rho, \tag{3.26}$$

from which we find

$$\theta = (ic/\rho)TT', \tag{3.27}$$

$$k = (\eta - il)/(\xi + il), \tag{3.28}$$

where c and l are integration constants. By substituting Eqs. (3.29) into Eqs. (3.9), we obtain

$$u = \frac{k+1}{4\rho\theta}\left[\theta - 1 \pm \left(\theta^2 - 2\frac{k-1}{k+1}\theta + 1\right)^{\frac{1}{2}}\right],$$
$$v = \frac{k+1}{4\rho k\theta}\left[\theta + 1 \pm \left(\theta^2 - 2\frac{k-1}{k+1}\theta + 1\right)^{\frac{1}{2}}\right]. \tag{3.29}$$

The third Bäcklund transformation is therefore

$$\partial_\xi E' = \frac{T'(k+1)}{2T\theta}\left[\theta^2 - \frac{2k}{k+1}\theta + 1 \pm (\theta - 1)(\theta^2 - 2\frac{k-1}{k+1}\theta + 1)^{1/2}\right]\partial_\xi E + \frac{T'(k+1)}{4\rho\theta} \times \left[\theta - 1 \pm (\theta^2 - 2\frac{k-1}{k+1}\theta + 1)^{1/2}\right],$$

$$\partial_\eta E' = -\frac{T'(k+1)}{2Tk\theta}\left[\theta^2 + \frac{2}{k+1}\theta + 1 \pm (\theta + 1)(\theta^2 - 2\frac{k-1}{k+1}\theta + 1)^{1/2}\right]\partial_\eta E + \frac{k+1}{4\rho k\theta}\left[\theta + 1 \pm (\theta^2 - 2\frac{k-1}{k+1}\theta + 1)^{1/2}\right], \tag{3.30}$$

where θ and k are defined by Eqs. (3.27) and (3.28) respectively.

4. PSEUDOPOTENTIALS

The Bäcklund transformations obtained in the previous sections have very complex forms. They, however, are rewritten in more simple forms by introducing appropriate pseudopotentials.[9] In this section we define the associated pseudopotentials with the Bäcklund transformations.

(i) When we take f given by Eq. (3.14) as the pseudopotential φ_1, the transformation (3.16) can be written as

$$\partial_\xi E' = (T'/T)\varphi_1\partial_\xi E, \quad \partial_\eta E' = (T'/T)\varphi_1\partial_\eta E, \tag{4.1}$$

where $\varphi_1\bar{\varphi}_1 = 1$, and satisfies

$$\partial_\xi\varphi_1 = \frac{\varphi_1 - 1}{2T}(\varphi_1\partial_\xi E + \partial_\xi\bar{E}),$$
$$\partial_\eta\varphi_1 = \frac{\varphi_1 - 1}{2T}(\varphi_1\partial_\eta E + \partial_\eta\bar{E}). \tag{4.2}$$

This is essentially equivalent to the I_1 transformations of Neugebauer.[10]

(ii) When we take f given by (3.19) as the pseudopotential φ_2, the second Bäcklund transformation (3.23) becomes

$$\partial_\xi E' = \frac{T'}{T}\varphi_2\partial_\xi E + \frac{T'}{2\rho}(1-\varphi_2),$$
$$\partial_\eta E' = \frac{T'}{T}\frac{1}{\varphi_2}\partial_\eta E + \frac{T'}{2\rho}\frac{\varphi_2 - 1}{\varphi_2}, \qquad (4.3)$$

where φ_2 is real and satisfies

$$\partial_\xi \varphi_2 = -[(\varphi_2-1)/4T]\,[(\varphi_2+1)(\partial_\xi E + \partial_\xi \bar{E}) + (\varphi_2 - 1)(\partial_\xi E - \partial_\xi \bar{E})] + (1/4\rho)(\varphi_2 - 1)(\varphi_2+1),$$
$$\partial_\eta \varphi_2 = -[(\varphi_2-1)/4T]\,[(\varphi_2+1)(\partial_\eta E + \partial_\eta \bar{E}) - (\varphi_2 - 1)(\partial_\eta E - \partial_\eta \bar{E})] + (1/4\rho)(\varphi_2 - 1)(\varphi_2+1). \qquad (4.4)$$

This Bäcklund transformation is equivalent to the I_2 transformation of Neugebauer.

(iii) We define the pseudopotential φ_3 associated with the transformation (3.30) as

$$\theta = -(k+1)\varphi_3/(\sqrt{-k}\,\varphi_3 + 1)(\varphi_3 + \sqrt{-k}\,); \qquad (4.5)$$

then the third Bäcklund transformation is found to have following form:

$$\partial_\xi E' = -\frac{T'}{T}\frac{\varphi_3(\sqrt{-k}\,\varphi_3+1)}{\varphi_3+\sqrt{-k}}\partial_\xi E + \frac{T'}{2\rho}(\sqrt{-k}\,\varphi_3+1),$$
$$\partial_\eta E' = -\frac{T'}{T}\frac{\sqrt{-k}\,\varphi_3+1}{\varphi_3(\varphi_3+\sqrt{-k}\,)}\partial_\eta E + \frac{T'}{2\rho\sqrt{-k}\,\varphi_3}(\sqrt{-k}\,\varphi_3+1). \qquad (4.6)$$

In addition we can show that φ_3 satisfies

$$\partial_\xi \varphi_3 = (1/2T)\left[\varphi_3(\sqrt{-k}\,\varphi_3+1)\partial_\xi E - (\varphi_3+\sqrt{-k}\,)\partial_\xi \bar{E}\,\right] - (\sqrt{-k}\,/4\rho)(\varphi_3-1)(\varphi_3+1),$$
$$\partial_\eta \varphi_3 = (1/2T\sqrt{-k}\,)\left[-(\sqrt{-k}\,\varphi_3+1)\partial_\eta E + \varphi_3(\varphi_3+\sqrt{-k}\,)\partial_\eta \bar{E}\,\right] - (1/4\sqrt{-k}\,\rho)(\varphi_3-1)(\varphi_3+1). \qquad (4.7)$$

This is equivalent to the Bäcklund transformation of Harrison.

5. CONCLUSION AND DISCUSSIONS

By using the method of Clairin we have obtained the four kinds of Bäcklund transformations for the Ernst equation. These transformations are equivalent to the transformations given by Ehlers, Neugebauer, and Harrison. It is clear that the Bäcklund transformation is not unique. We have assumed the functional forms of P and Q as given in Eqs. (2.3). However, we have observed that Eqs. (2.3) are general enough to cover all the known transformations.

Recently Belinsky–Zakharov, Maison, and Hauser–Ernst have shown the existence of linear eigenvalue problems in the spirit of Lax.[11] There, the Ernst equation arises as the compatibility condition for the linear eigenvalue problem. In the theory of solitons, it has been known that the Bäcklund transformation and the inverse scattering method are closely related.[12] Then, it is a very interesting problem to clarify the relations between the Bäcklund transformations found in this paper and the inverse scattering problems discussed by Belinsky–Zakharov, Maison, and Hauser–Ernst. This problem is left for a future study.

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Inverse scattering connections

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We establish and study a transformation which connects the Schrödinger, the Klein–Gordon, and the Dirac operators. This provides an equivalence between their associated direct and inverse problems, and inverse spectral transforms.

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I. INTRODUCTION

We study here the relations that connect the Schrödinger,[1] Klein–Gordon[2] and Dirac[3] inverse problem (IP) and inverse scattering (or spectral) transforms (IST).

Some of the arguments have been previously sketched,[4] with the result that there exists a transformation relating the two couples (r,q) and (U,Q) of potentials of the Dirac and Klein–Gordon systems[5]:

$$(D):\left\{\partial_x + i\epsilon E\sigma_3 - \begin{pmatrix} 0 & q(x) \\ r(x) & 0 \end{pmatrix}\right\} Y^{\epsilon}(k,x)=0,\ \begin{cases} q(x) \underset{\pm\infty}{\sim} m \\ r(x) \underset{\pm\infty}{\sim} m \end{cases}, \tag{I.1}$$

$$(K):\left\{\partial_x^2 + k^2 - U(x) - \epsilon E Q(x)\right\} y^{\epsilon}(k,x)=0,\ \begin{cases} U(x) \underset{\pm\infty}{\sim} 0 \\ Q(x) \underset{\pm\infty}{\sim} 0 \end{cases}, \tag{I.2}$$

where the momentum k is related to the energy ϵE by $k^2=E^2-m^2$, and where $\epsilon=\pm$. It is shown here that the transformation gives a complete equivalence between IP and IST associated with (D) and (K). We show moreover that the well-known IP and IST for the Schrödinger equation:

$$(S):\left\{\partial_x^2 + k^2 - U(x)\right\} z(k,x)=0,\quad U(x) \underset{\pm\infty}{\sim} 0, \tag{I.3}$$

can be derived from (K), and thus from (D) too.

II. THE INVERSE PROBLEMS

We first have to come back to the procedure and formalism of IP which is already well known for $(S)^1$: let $\mathscr{S}_S$ be the set of spectral data

$$\mathscr{S}_S = \left\{R_S(k),\ k\in\mathbb{R};\ k_{n,S},\ (\operatorname{Im}k_{n,S}>0), C_{n,S},\ n=1,\ldots,N_S\right\}, \tag{II.1}$$

define the "Fourier transform" of $\mathscr{S}_S$ as

$$H_S(u)=\frac{1}{2\pi}\int_{-\infty}^{+\infty} dk\, R_S(k)e^{iku} - i\sum_{1}^{N_S} C_{n,S}\exp(ik_{n,S}u), \tag{II.2}$$

compute then the kernel $S(x,y)$ from $H_S(x+y)$ out of the Marchenko equation:

$$S(x,y) + H_S(x+y) + \int_x^{+\infty} du\, S(x,u)\, H_s(u+y) = 0 \quad \text{for } y>x. \tag{II.3}$$

The potential $U(x)$ is finally obtained by

$$U(x) = -2\, d_x S(x,x). \tag{II.4}$$

Here, and in the following, we do not deal with the problem of giving conditions on the spectral data so that the Marchenko equations do possess a (unique) solution which leads effectively to a potential.[6] The interested reader may refer to Ref. 1 for (S), Ref. 5 for (D) and Ref. 7 for (K).

In the (D) case, the eigenvalue is ϵE but we prefer to work with momentum k. Then ϵE appears as a double-valued function of k. The choice of the determination of the square root of k^2+m^2 makes k varying on a two-fold Reiman surface (cut from im to $i\infty$, and from $-im$ to $-i\infty$), each sheet of which is indexed by the sign ϵ of the real part of ϵE. The spectral data are:

$$\mathscr{S}_D = \left\{R_D^{\epsilon}(k),\ k\in\mathbb{R};\ k^{\epsilon}_{n,D}(\operatorname{Im}k^{\epsilon}_{n,D}>0),\ C^{\epsilon}_{n,D},\ n=1,\ldots,N^{\epsilon}_D,\ \epsilon=\pm\right\}, \tag{II.5}$$

with the Fourier transform:

$$H_D(u) = \sum_{\epsilon}\left\{\frac{1}{4\pi}\int_{-\infty}^{+\infty}\frac{dk}{\epsilon E}\begin{pmatrix} -im & -\epsilon E + k \\ \epsilon E + k & -im \end{pmatrix} R^{\epsilon}_D(k) e^{iku} - i\sum_{n=1}^{N^{\epsilon}_D}\frac{e^{iku}}{2\epsilon E}\begin{pmatrix} -im & -\epsilon E + k \\ \epsilon E + k & -im \end{pmatrix}\Bigg|_{k=k^{\epsilon}_{n,D}} C^{\epsilon}_{n,D}\right\} \tag{II.6}$$

The matrix Marchenko system reads

$$D(x,y) + H_D(x+y) + \int_x^{+\infty} du\, D(x,u) H_D(u+y) = 0 \quad \text{for } y>x, \tag{II.7}$$

and the potentials r and q are obtained from $D(x,x)$ by (we write another useful relation)

$$[\sigma_3, D(x,x)] = \begin{pmatrix} 0 & -(q-m) \\ r-m & 0 \end{pmatrix},$$
$$[\sigma_3, \sigma_1 D(x,x)] = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\int_x^{+\infty} (rq - m^2). \tag{II.8}$$

The (K) case is a little more complicated and we shall see that it is an interesting aspect of the above-mentioned transformation in that it provides an easier way to solve the IP for (K). The set of spectral data is defined like $\mathscr{S}_D$ by

$$\mathscr{S}_K = \left\{R^{\epsilon}_K(k), k\in\mathbb{R}; k^{\epsilon}_{n,K}, (\operatorname{Im}k^{\epsilon}_{n,K}>0), C^{\epsilon}_{n,K}, n=1,\ldots,N^{\epsilon}_K, \epsilon=\pm\right\}. \tag{II.9}$$

As shown in Ref. 2, we need to define three types of

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Fourier transforms of $\mathcal{S}_K$, namely:

$$H_K^{(p)}(u)=\sum_\epsilon\left\{\frac{1}{4\pi}\int_{-\infty}^{+\infty}dk\,(\epsilon E)^{p-2}R_K^\epsilon(k)e^{iku}-\tfrac{1}{2}i\sum_{n=1}^{N_K^\epsilon}(\epsilon E)^{p-2}e^{iku}\Big|_{k=k_{n,K}^\epsilon}C_{n,K}^\epsilon\right\},\quad p=1,2,3.\quad \text{(II. 10)}$$

The Marchenko system of inversion equations reads: for $y>x$,

$$K_1(x,y)+F(x)H_K^{(2)}(x+y)+\int_x^{+\infty}du\,[K_1(x,u)H_K^{(2)}(u+y)-K_2(x,u)H_K^{(3)}(u+y)]=0,\quad \text{(II. 11)}$$

$$-K_2(x,y)+F(x)H_K^{(1)}(x+y)+\int_x^{+\infty}du\,[K_1(x,u)H_K^{(1)}(u+y)-K_2(x,u)H_K^{(2)}(u+y)]=0.\quad \text{(II. 12)}$$

[The function $F(x)$ is introduced to correct the asymptotic behaviors of the Jost solutions of (K) for large values of $|k|$ (see Refs. 2 and 7.)] The kernels $K_{1,2}$, solutions of (II. 11) and (II. 12), lead to potentials $U(x)$ and $Q(x)$ via

$$-d_x^2F(x)+U(x)F(x)+2d_xK_1(x,x)+Q(x)\partial_uK_2(x,u)\Big|_{u=x}=0,\quad \text{(II. 13)}$$

$$Q(x)F(x)-2d_xK_2(x,x)=0\ ,\quad \text{(II. 14)}$$

$$2d_xF(x)+Q(x)K_2(x,x)=0\ .\quad \text{(II. 15)}$$

III. CONNECTION OF DIRECT SCATTERING PROBLEMS

A. Connection of (D) with (K)

We now wish to transform the system of two coupled first order differential Equations (I. 1) into a second order differential equation of type (I. 2). The relation that we search for is obviously

$$Y^\epsilon(k,x)=\alpha^\epsilon(k)\begin{pmatrix}a^\epsilon(m;k,x) & b^\epsilon(m;k,x)\\ c^\epsilon(m;k,x) & d^\epsilon(m;k,x)\end{pmatrix}\begin{pmatrix}y^\epsilon(k,x)\\ y_x^\epsilon(k,x)\end{pmatrix},\quad \text{(III. 1)}$$

where the functions $a, b, c,$ and d remain to be defined (subscript x means partial derivative with respect to x). We shall now omit ϵ and recall it whenever necessary.

In Ref. 4 we computed $a, b, c,$ and d by demanding that the transformed equation [obtained by inserting (III. 1) into (I. 1)] is the (K) equation. For the purpose of getting more information, we start with the assumption that the equation governing $y(k,x)$ belongs to a set of scattering problems which possess the same spectral data as (D). [The word *same* is taken in the sense of

$$T_D(k)=T_K(k)\quad \text{for } \mathrm{Im}(k)\geq 0.]\quad \text{(III. 2)}$$

The result is

Theorem 1: In the case of q and r going asymptotically to the same constant m, the Klein–Gordon equation is the only second order differential equation which possesses the same spectral data as the Dirac equation.

Proof: We may first exploit the compatibility condition [which is that $Y(k,x)$ is a solution (D)], expressed in the fact that $y(k,x)$ becomes a solution of a system of two second order differential equations. These two equations must be linearly dependent; therefore

$$d=vb,\quad \text{(III. 3)}$$

$$v(a+b_x+iEb-qd)=c+d_x-iEd-rb,\quad \text{(III. 4)}$$

$$v(a_x+iEa-qc)=c_x-iEc-ra,\quad \text{(III. 5)}$$

$v(x)$ being an arbitrarily choosen function. The other relation needed to solve this system is obtained from (III. 2). One has to use the definitions of the Jost solutions (and spectral data) of (D) and (K), (the reader may refer to Refs. 2 and 3 whose notations are employed here), to see that (III. 2) reads:

$$|\phi(k,x),\ \psi(k,x)|=W(g(k,x),f(k,x))(1/2ik).\quad \text{(III. 6)}$$

[The symbol $|\phi,\psi|$ denotes the determinant of the matrix of the column vectors ϕ and ψ, and $W(f,g)$ is the Wronskian of functions f and g.] By inserting now (III. 1) into (III. 6), one gets a necessary condition to achieve (III. 2):

$$\partial_x(ad-bc)=0\ .\quad \text{(III. 7)}$$

Let us insert (III. 7) into (III. 4) and make use of (III. 3) to get

$$bd[-2iE+v_x/v+qv-r/v]=\text{const.}\quad \text{(III. 8)}$$

Taking advantage of the fact that (III. 8) holds for $\epsilon=\pm$, (that is, for $\pm E$), we may write

$$bd=1,\quad v_x/v+qv-r/v=Z\ ,\quad \text{(III. 9)}$$

where Z is an arbitrary constant. We have set $bd=1$, which simply corresponds to an adjustment of $\alpha(k)$ in (III. 1). Hence (III. 3) gives

$$d=v^{1/2},\quad b=v^{-1/2}\ .\quad \text{(III. 10)}$$

A little algebra applied to the system (III. 4) and (III. 5), changes it into a Kramer system for a and c, the solution of which is

$$a=v^{-1/2}[-iE+Z/2+w]\ ,\qquad c=v^{1/2}[iE+Z/2+w]\ ,\quad \text{(III. 11)}$$

where

$$2w=qv+r/v\ .\quad \text{(III. 12)}$$

At this point, the mapping (III. 1) is completely determined: for given r and q, first solve the Ricatti equation (III. 9) for $v(x)$;[8] then obtain $a, b, c,$ and d from (III. 10) and (III. 11).

Inserting now (III. 1) into (D) with the above definitions of functions $a, b, c,$ and d, we are led to a Klein–Gordon type equation for $y(k,x)$:

$$\left\{\partial_x^2+(k^2+Z^2/4)-(w^2-w_x-m^2)+(E+iZ/2)iv_x/v\right\}y(k,x)=0.\quad \text{(III. 13)}$$

The final step of this proof consists of assuming that the potentials that appear in (III.13), namely

$$U = w^2 - w_x - m^2, \quad Q = -iv_x/v, \tag{III.14}$$

approach zero asymptotically. This implies in particular that $v(x) \underset{\pm\infty}{\simeq} 1$. Thus we can see from Equation. (III.9) that, in the case of $q(x)$ and $r(x)$ going asymptotically to the same constant m, we have $Z=0$, and (III.13) is nothing but (K). We shall denote by $\mathfrak{F}$ the transformation $(r,q) \to (U,Q)$ defined by (III.9) for $Z=0$, (III.12), and (III.14).

To end this section, we give below the whole relation between $\mathscr{S}_D$ and $\mathscr{S}_K$ induced by assumption (III.2), (the proof of the following statements can be found in Ref. 4). (III.2) implies that both (D) and (K) have the same bound states:

$$k_{n,D} = k_{n,K}, \quad N_D = N_K, \tag{III.15}$$

and we have[4]

$$R_D(k) = \frac{\alpha(k)}{\alpha(-k)} R_K(k), \quad \alpha(k) = \left(\frac{E+k}{2k}\right)^{1/2} \frac{i}{E+k+im}, \tag{III.16}$$

$$C_{n,D} = \left.\frac{\alpha(k)}{\alpha(-k)}\right|_{k=k_n} C_{n,K}. \tag{III.17}$$

B. Connection of (D) and (K) with (S)

It seems clear that, setting $Q=0$ and $m=0$ in (K), $\mathscr{S}_K$ must reduce to $\mathscr{S}_S$. The proof is not obvious and we work it out by using (D) as an intermediary [note that, for $m=0$, (D) reduces to the Zakharov–Shabat system (ZS)[9,10]]. Writing (III.16) and (III.17) for $m=0$, and remembering that $E=k$ for $\mathrm{Re}(k) \geq 0$, and $E=-k$ for $\mathrm{Re}(k)<0$, we find

$$\begin{aligned} &R_D^+(k) = -R_K^+(k), \; R_D^-(k) = R_K^-(k) \text{ for } \mathrm{Re}(k) \geq 0, \; m=0, \\ &R_D^+(k) = R_K^+(k), R_D^-(k) = -R_K^-(k) \text{ for } \mathrm{Re}(k) < 0, \; m=0. \end{aligned} \tag{III.18}$$

But for $Q=0$, the solution of $\mathfrak{F}$ is $r=q$, and we may use the results of Ref. 9 together with the particular properties of the spectral data of (ZS) induced by $r=q$ [see Ref 10 formula (4.24), p. 271], to get

$$R_D^+(k) = -R_D^-(k) \text{ for all real } k \text{ (and } m=0). \tag{III.19}$$

Therefore

$$R_K^+(k) = R_K^-(k) \text{ for all real } k \text{ (and } m=0), \tag{III.20}$$

and this reflection coefficient is nothing other than $R_S(k)$. The same procedure holds for the transmission coefficient $T_K(k)$ and the normalization constants $C_{n,K}$:

$$T_K^+(k) = T_K^-(k) = T_S(k), \quad N_K^+ = N_K^- = N_S, \quad C_{n,K}^+ = C_{n,K}^- = C_{n,S}. \tag{III.21}$$

On the other hand, these statements lead to a connection between (ZS) and (S) spectral problems

Corollary 1: for $r=q$, (ZS) is equivalent to (S) for the potential[11]

$$U = q^2 - q_x. \tag{III.22}$$

The corresponding relations among the spectral data are readily given by (III.18), where one replaces $R_K(k)$ by $R_S(k)$. In contrast to the case $r=-1$, (see Ref. 10, Appendix 3) the transformation (III.22) is not singular.

IV. CONNECTION OF INVERSE PROBLEMS

A. Connection of IP for (D) with IP for (K)

(D) and (K) having the same spectral data, and their potentials being related by $\mathfrak{F}$, we may state

Theorem 2: the solution of the IP for (K) consists in first solving IP for (D) and then obtaining (U,Q) from (r,q).

The proof of Theorem 2 will be concluded if it is shown that the inversion equations (II.8) for (D) are equivalent to equations (II.13), (II.14), and (II.15) for (K). For this purpose we look for a set of relations which connect the kernels $K_1(x,y)$ and $K_2(x,y)$ to the matrix kernel $D(x,y) = \begin{pmatrix} D_1 & D_2 \\ D_3 & D_4 \end{pmatrix}$. This is done with the help of the definitions of these kernels from the Jost solutions of (D) and (K) respectively:

$$\psi(k,x) = \left[e^{ikx} + \int_x^{+\infty} dy\, D(x,y) e^{iky}\right] \begin{pmatrix} 1 \\ \dfrac{im}{E+k} \end{pmatrix} \left(\frac{E+k}{2k}\right)^{1/2}, \tag{IV.1}$$

$$f(k,x) = F(x)e^{ikx} + \int_x^{+\infty} dy\,[K_1(x,y) - EK_2(x,y)]e^{iky} \tag{IV.2}$$

We compute the quantity

$$-i\left(\frac{2k}{E+k}\right)^{1/2}\Big[(E+k+im)\psi(-k,x)e^{ikx} - (E+k-im) \times \psi(k,x)e^{-ikx}\Big]$$

on one hand with the help of (IV.1), on the other hand through (III.1) and (IV.2). We use partial integration techniques to eliminate all the terms containing k as a factor, and keep in mind the fact that all the results are valid for $\epsilon = \pm$. On calculating, we arrive at two sets of four relations which arise from a vectorial equation of the type

$$A(x,x) + \epsilon EB(x,x) + \int_x^{+\infty} dy \cos(k(x-y)) \times [A'(x,y) + \epsilon EB'(x,y)] = 0, \tag{IV.3}$$

valid for all k and ϵ. The solution is $A = A' = B = B' = 0$, namely

$$F(x) + iK_2(x,x) = v(x)^{1/2}, \tag{IV.4a}$$

$$F(x) - iK_2(x,x) = v(x)^{-1/2}, \tag{IV.4b}$$

$$\left. w(x)F(x) + d_xF(x) - K_1(x,x) - i\partial_u K_2(x,u)\right|_{u=x} = v(x)^{1/2}(m - D_1(x,x) - D_2(x,x)), \tag{IV.4c}$$

$$\left. w(x)F(x) + d_xF(x) - K_1(x,x) + i\partial_u K_2(x,u)\right|_{u=x} = v(x)^{-1/2}(m - D_3(x,x) - D_4(x,x)), \tag{IV.4d}$$

$$(m-\partial_y)(D_1(x,y)+D_2(x,y))$$
$$=(\partial_x+w(x))K_1(x,y)+i(m^2-\partial_y^2)K_2(x,y)\ , \qquad \text{(IV.5a)}$$

$$(m-\partial_y)(D_3(x,y)+D_4(x,y))$$
$$=(\partial_x+w(x))K_1(x,y)-i(m^2-\partial_y^2)K_2(x,y)\ , \qquad \text{(IV.5b)}$$

$$D_1(x,y)-D_2(x,y)=K_1(x,y)-i(\partial_x+w(x))K_2(x,y)\ , \qquad \text{(IV.5c)}$$

$$D_3(x,y)-D_4(x,y)=-K_1(x,y)-i(\partial_x+w(x))K_2(x,y)\ . \qquad \text{(IV.5d)}$$

It is obvious that the system (IV.4a) and (IV.4b), with $v(x)=\exp(-i\int_x^{+\infty}du\,Q(u))$, is nothing other than the system (II.14) and (II.15). The following step consists of replacing the D_i's by their expressions given by (II.8), computing the quantities $\partial_u K_2(x,u)|_{u=x}$ and $K_1(x,x)$ from (IV.4c) and (IV.4d), inserting the results into (II.13), and finally verifying that (II.13) holds. Therefore the system (IV.4) is equivalent to the system (II.13), (II.14), and (II.15), which concludes the proof of Theorem 2.

One could show, moreover, that the system of partial differential equations (IV.5), together with the Cauchy conditions (IV.4), defines completely the relations between the kernels $D(x,y)$ and $K_{1,2}(x,y)$. Let us finally notice that for $Q=0$, (and thus for $r=q$) the system (IV.4c) and (IV.4d) gives rise to the transformation (III.22).

B. Connection of IP for (*K*) and (*D*) with IP for (*S*)

We now wish to show the following statement:

Corollary 2: in the case of Q and m being zero, the IP for (K) reduces to the IP for (S).

Proof: First, one can readily verify from (III.20) that the Fourier transform (III.10) of $\mathscr{S}_K$ reduces to

$$H_K^{(1)}(u)=0,\quad H_K^{(2)}(u)=H_S(u),\quad H_K^{(3)}(u)=0. \qquad \text{(IV.6)}$$

Second, for $Q=0$, the solution of (II.14) and (II.15) is

$$F(x)=1,\quad K_2(x,x)=0\ . \qquad \text{(IV.7)}$$

We now write the system (IV.4c) and (IV.4d) for $r=q$, that is to say, for $D_1(x,x)=D_4(x,x)$ and $D_2(x,x)=D_3(x,x)$, and obtain

$$\partial_u K_2(x,u)|_{u=x}=0\ . \qquad \text{(IV.8)}$$

Thus Eq. (II.13) reduces to (II.4). We now have to verify that the system (II.11) and (II.12) does become the Marchenko equation (II.3). $K_2(x,y)$ is the solution of

$$K_2(x,y)+\int_x^{+\infty}du\,K_2(x,u)H_S(u+y)=0\quad\text{for } y>x, \qquad \text{(IV.9)}$$

with the initial condition (IV.7). This solution is thus assumed to be[12]

$$K_2(x,y)=0\ , \qquad \text{(IV.10)}$$

and Eq. (II.11) reads like (II.3) for $S(x,y)=K_1(x,y)$.

V. THE INVERSE SPECTRAL TRANSFORMS

We shall now discuss some consequences of the above results for the IST method. This method consists essentially of assuming that the initial data [say $U(x,0)$] of a nonlinear evolution problem is the potential of some scattering problem (the form of the solvable nonlinear problem depends directly on the chosen scattering problem). One may then obtain the spectral data at t [see, for example, Eq. (V.8) below] and get $U(x,t)$ through the inverse problem. Let us now recall the way IST works in the three cases considered. The IP for (S) allows us to solve the following nonlinear evolution equations (NEE)[1,13]:

$$\{\partial_t+\Lambda(S^+)\partial_x\}\,U(x,t)=0\ , \qquad \text{(V.1)}$$

in which $\Lambda(k^2)$ is an entire function of k^2 and S^+ is the operator

$$S^+=-\tfrac14\partial_x^2+U-\tfrac12U_xI\ . \qquad \text{(V.2)}$$

Here and in the following, the operator I is defined by its action on a generic function $f(x,t)$ as

$$If(x,t)=\int_x^{+\infty}dy\,f(y,t)\ . \qquad \text{(V.3)}$$

When using the results of IP for (K), one may solve[2]

$$\{\partial_t+\Lambda(K^+)\partial_x\}\begin{pmatrix}U(x,t)\\Q(x,t)\end{pmatrix}=0\ , \qquad \text{(V.4)}$$

where Λ is now an entire function of ϵE and K^+ is given by

$$K^+=\begin{pmatrix}0 & S^++m^2\\ 1 & Q-\tfrac12Q_xI\end{pmatrix}\ . \qquad \text{(V.5)}$$

Finally, if one uses IP for (D), one will find the following set of solvable NEE[3]:

$$\{\partial_t+\Lambda(D^+)\partial_x\}\begin{pmatrix}r(x,t)\\-q(x,t)\end{pmatrix}=0\ , \qquad \text{(V.6)}$$

Λ being an entire function of ϵE and D^+ being defined by

$$2iD^+=\begin{pmatrix}\partial_x+2rIq & -2rIr\\ 2qIq & -\partial_x-2qIr\end{pmatrix}\ . \qquad \text{(V.7)}$$

There is not much to say about the connection between IST for (K) and IST for (D); the transformation $\mathfrak{F}$ previously defined makes no explicit reference to the time dependence. There thus exists a one-to-one correspondence betweeen solutions of NEE (V.4) and (V.6), especially as (K) and (D) possess the same spectral data, which both evolves according to

$$\{\partial_t+2ik\Lambda(E)\}R(k,t)=0,\ \ \partial_tT(k,t)=0,\ \ \{\partial_t+2ik_n\Lambda(E_n)\}C_n(t)=0. \qquad \text{(V.8)}$$

But we must pause a moment to look into the case $Q=0$ (or equivalently $r=q$), for indeed we shall prove that:

Theorem 3: in the case $Q=0$, the IST formalism for the (K) eigenvalue problem remains valid only when $\Lambda(E)$ is an even function of E.

In order to see this, let us consider the NEE (V.4) for $Q=0$ and for $\Lambda(E)=E^{2N+1}$; it reads

$$\begin{pmatrix}U_t\\0\end{pmatrix}=\begin{pmatrix}0 & S^+\\1 & 0\end{pmatrix}^{2N+1}\begin{pmatrix}U\\0\end{pmatrix}, \qquad \text{(V.9)}$$

which leads to

$$\begin{pmatrix} U_t \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ [S^{-}]^N U \end{pmatrix} \qquad (V.10)$$

Therefore $U(x,t)$ does not evolve in time, which proves Theorem 3.

Furthermore, in the case $m=0$, when Λ possesses an odd part (say Λ_0) the relation (III.20) does not hold anymore for $t\neq 0$; indeed we have

$$R_K^{\pm}(k,t) = R_S(k,0)\exp[-2ik(\Lambda_e \pm \Lambda_0)t]\,. \qquad (V.11)$$

One can thus readily find out that the Marchenko equations (II.11) and (II.12) have no solution, since (V.11) implies that (IV.6), and thus (IV.10), are no longer valid.

Note that Theorem 3 becomes readily understandable if one takes account of the fact that the procedure of inversion for (S) works with Λ as an entire function of k^2, that is, and even (entire) function of k.

Another argument for completing the proof of Theorem 3 can be found in the study of particular solutions of NEE (V.6), named solitons, obtained by assuming that the input data $(r(x,0), q(x,0))$ possess a set of spectral data reduced to a discrete spectrum only. The derivation of such a soliton solution is given in Ref. 3, the result of which is:

for $R_D(k)=0$, $N_D^+ = N_D^- = 1$, $k^+_{n,D} = k^-_{n,D} = iu$, $(0<u<m)$, $C_D^+(0) = -C_D^-(0) = C$, we found

$$q(x,t) - m = 2u\,\frac{(u/E+i)\exp[2u\Lambda_0 t] + (u/E-i)\exp[-2u\Lambda_0 t]}{\cosh[2u(x-x_0-\Lambda_e t-\lambda)]}, \qquad (V.12)$$

$$r(x,t) - m = 2u\,\frac{(u/E-i)\exp[2u\Lambda_0 t] + (u/E+i)\exp[-2u\Lambda_0 t]}{\cosh[2u(x-x_0-\Lambda_e t-\lambda)]}, \qquad (V.13)$$

where $E^2 = m^2 - u^2$ and $\lambda = (1/2u)\ln(C/2u)$. It is clear from (V.12) and (V.13) that to get $r=q$ one must set $\Lambda_0 = 0$.

It will be of interest to compare (V.12), as an example for $\Lambda = -4E^2$, solution of the modified Korteveg–de Vries equation:

$$q_t + q_{xxx} - 6q^2 q_x + 2m^2 q_x = 0\,, \qquad (V.14)$$

to the corresponding solution of equation (V.4), which reads in that very case:

$$U_t + U_{xxx} - 6UU_x - 4m^2 U_x = 0\,. \qquad (V.15)$$

The interest in such a comparison is that, for the above chosen set of spectral data, $q(x,t)$ given by (V.12) is a soliton that comes back (often called boomeron[14]). But the Korteveg–de Vries equation (V.15) is known not to possess reflected solutions and thus the transformation (III.22) will change a boomeron into a soliton. Let us now compute this soliton solution of (V.15); we shall not repeat the procedure, which is exactly the same as in the (S) case[1] with the only difference being that $\Lambda(E)$ is now $-4(m^2-u^2)$ in spite of $4u^2$. Nevertheless, one may pay attention to the relation between C_K^+ and C_K^- induced by the assumption $C_D^+(0) = -C_D^-(0)$. Using definition of the normalization constants C (see for example Ref. 2), and the relation (III.16), one shows that

$$C_D^+(0)/C_D^-(0) = -C_K^+(0)/C_K^-(0)\,, \qquad (V.16)$$

and therefore

$$C_K^+(0) = C_K^-(0)\,. \qquad (V.17)$$

This is the expected result. Indeed, the same arguments as those employed in the proof of Theorem 3 lead us to choose a set of spectral data so that the system of Marchenko equation (II.11) and (II.12) does reduce to (II.2), that is to say, so that (IV.6) holds. For the given set of spectral data, the relation (V.17) is the condition which ensures that (IV.6) holds.[15]

The solution of (V.15) is, finally

$$U(x,t) = 2u^2\sinh^{-2}[u(x-4(u^2-m^2)t-\lambda')]\,, \qquad (V.18)$$

where $\lambda' = (1/2u)\ln(C'/2u)$, and C' is the normalization constant (V.17). For $m=0$, one finds the one-soliton solution of the KdV equation. The m^2 term simply corresponds to a translation of the coordinate system at speed $4m^2$. can be verified directly on (V.15): by setting

$$\partial_\tau = \partial_t - 4m^2\partial_x\,, \qquad (V.19)$$

one gets the usual KdV equation for $U(x,\tau)$.[16]

[1]For the one-dimensional IP see L. D. Fadeev, Dokl. Akad. SSSR **121**, 63 (1958), and also Z. S. Agranovich and V. A. Marchenko, *The Inverse Problem of Scattering Theory* (Gordon and Breach, New York (1963); for the associated IST, see C. S. Gardner, J. M. Greene, M. D. Kruskal, and R. M. Miura, Commun. Pure Appl. Math. **27**, 97 (1974).

[2]The IP is solved in J. JP. Leon, Lett. Nuovo Cimento **29**, 45 (1980) and the IST in J. JP. Leon, Nuovo Cimento **28**, 107 (1980).

[3]J. JP. Leon, J. Math. Phys. **21**, 2572 (1980).

[4]J. JP. Leon, Lett. Math. Phys. **5**, 1 (1981); for the $m=0$ case, see M. Jaulent and I. Miodek, Lett. Nuovo Cimento **20**, 655 (1977).

[5]In Ref. 3 we studied the more general case $r(x)\underset{\pm\infty}{\sim} r^{\pm}$ and $q(x)\underset{\pm\infty}{\sim} q^{\pm}$, with the constraint $r^+q^+ = r^-q^- = m^2$. We shall not work here with this generalization, which would unnecessarily complicate the results.

[6]This problem is partially solved in the radial case by M. Gasimov and B. M. Levitan, Dokl. Akad. Nauk. SSSR **167** (1966).

[7]For the case $Q=2V$ and $U=-V^2$, see R. Weiss and G. Scharf, Helv. Phys. Acta **44**, 910 (1971), and H. Cornille, J. Math. Phys. **11**, 79 (1970).

[8]The technique of solution of (II.9) is given in Ref. 4.

[9]The complete relation between Jost solutions and spectral data of (*D*) with $m=0$ and (ZS) problems is given in the unpublished work by J. JP. Leon, "Thèse de Doctorat de Troisième Cycle," U. S. T. L., Montpellier (June 1978).

[10]M. J. Ablowitz, D. J. Kaup, A. C. Newell, and H. Segur, Stud. Appl. Math. **53**, 249 (1974).

[11]Relation (III.22) is, for $m=0$, the Miura transformation, R. M. Miura, J. Math. Phys. **9**, 1202 (1968).

[12]As said before, we always suppose that such Fredholm equations [as (IV.9)], have a unique solution.

[13]A general survey of the theory of IST may be found in M. J. Ablowitz, Stud. Appl. Math. **58**, 17 (1978).

[14]This denomination has been introduced by F. Calogero and A. Degasperis, Nuovo Cimento **39 B**, 1 (1977).

[15]These arguments are in fact the *a posteriori* reason why we chose $C^+(0) = -C^-(0)$ in Ref. 3.

[16]Thanks are due to Dr. J. C. Fenandez for valuable comments concerning this point.

Symmetries and the Dirac equation

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A new class of symmetries are given for the Dirac equation without external fields. We consider the two cases of massive and massless particles.

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1. INTRODUCTION

It is convenient to divide the class of transformation groups in Lie tangent transformation groups[1] and Lie–Bäcklund tangent transformation groups.[2] In a previous paper[3] one of the authors has investigated Lie–Bäcklund tangent transformation groups for Maxwell's equations in the absence of sources. The infinitesimal operators have been given.

In the present paper we investigate the Dirac equation without external fields and infinitesimal symmetries. We consider three cases: the Dirac equation without rest mass, the Dirac equation with rest mass, and the Dirac equation with a nonlinearity $\psi(\bar{\psi}\psi)$.

It is well known that the Dirac equation with zero rest mass admits the 15-parameter conformal group which contains the 10-parameter Poincaré group. In the following such transformations (sometimes called transformations of geometrical type) are not considered. Rather we study infinitesimal symmetries of the type $\sum_i \eta_i(\phi)\partial/\partial\phi_i$, where $\phi_i(x)$ $(i=1,\ldots,m)$ denotes the field under consideration and $x\equiv(x_1,x_2,x_3,x_4)$ $(x_4\equiv ct)$. Moreover, we consider Lie–Bäcklund tangent transformation groups.

2. DIRAC EQUATION WITH VANISHING REST MASS

The Dirac equation with vanishing rest mass is given by the following linear system of partial differential equations:

$$\sum_{k=1}^{3}\hbar\frac{\partial}{\partial x_k}(\gamma_k\psi)-i\hbar\frac{\partial}{\partial x_4}(\gamma_4\psi)=0, \tag{2.1}$$

where $x_4\equiv ct$ and $\psi\equiv(\psi_1,\psi_2,\psi_3,\psi_4)^T$ (T means transpose). γ_1, γ_2, γ_3, and γ_4 are the following 4×4-matrices

$$\gamma_1=\begin{bmatrix}0&0&0&-i\\0&0&-i&0\\0&i&0&0\\i&0&0&0\end{bmatrix};\quad \gamma_2=\begin{bmatrix}0&0&0&-1\\0&0&1&0\\0&1&0&0\\-1&0&0&0\end{bmatrix};$$
$$\gamma_3=\begin{bmatrix}0&0&-i&0\\0&0&0&i\\i&0&0&0\\0&-i&0&0\end{bmatrix};\quad \gamma_4=\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&-1\end{bmatrix}. \tag{2.2}$$

From Eq. (2.1) it follows that

$$\sum_{k=1}^{3}\frac{\partial}{\partial x_k}(\gamma_k\psi)-i\frac{\partial}{\partial x_4}(\gamma_4\psi)=0. \tag{2.3}$$

Let $x=(x_1,x_2,x_3,x_4)$. Since $\psi_k(x)$ $(k=1,2,3,4)$ is a complex quantity we put $\psi_k(x)=u_k(x)+iv_k(x)$, where $u_k(x)$ and $v_k(x)$ are real fields. Then we obtain the following coupled system of eight linear partial differential equations

$$\begin{aligned}
&-\partial u_4/\partial x_1-\partial v_4/\partial x_2-\partial u_3/\partial x_3-\partial u_1/\partial x_4=0,\\
&-\partial u_3/\partial x_1+\partial v_3/\partial x_2+\partial u_4/\partial x_3-\partial u_2/\partial x_4=0,\\
&\partial u_2/\partial x_1+\partial v_2/\partial x_2+\partial u_1/\partial x_3+\partial u_3/\partial x_4=0,\\
&\partial u_1/\partial x_1-\partial v_1/\partial x_2-\partial u_2/\partial x_3+\partial u_4/\partial x_4=0,\\
&-\partial v_4/\partial x_1+\partial u_4/\partial x_2-\partial v_3/\partial x_3-\partial v_1/\partial x_4=0,\\
&-\partial v_3/\partial x_1-\partial u_3/\partial x_2+\partial v_4/\partial x_3-\partial v_2/\partial x_4=0,\\
&\partial v_2/\partial x_1-\partial u_2/\partial x_2+\partial v_1/\partial x_3+\partial v_3/\partial x_4=0,\\
&\partial v_1/\partial x_1+\partial u_1/\partial x_2-\partial v_2/\partial x_3+\partial v_4/\partial x_4=0.
\end{aligned} \tag{2.4}$$

The method for investigating the infinitesimal symmetries has been described by one of the authors.[3] Following Dieudonné[4] we cast the system of partial differential equations into an equivalent set of differential forms, where we put:

$$\begin{aligned}&\partial u_i/\partial x_j\to p_{ij}\\&\partial v_i/\partial x_j\to q_{ij}\end{aligned}\quad (i,j=1,2,3,4) \tag{2.5}$$

Consequently, for the investigation of infinitesimal symmetries we consider the following differential forms:

$$\begin{aligned}
&F_1(p_{11},\ldots,p_{44},q_{11},\ldots,q_{44})=-p_{41}-q_{42}-p_{33}-p_{14},\\
&F_2(\cdots\cdots)=-p_{31}+q_{32}+p_{43}-p_{24},\\
&F_3(\cdots\cdots)=p_{21}+q_{22}+p_{13}+p_{34},\\
&F_4(\cdots\cdots)=p_{11}-q_{12}-p_{23}+p_{44},\\
&F_5(\cdots\cdots)=-q_{41}+p_{42}-q_{33}+q_{14},\\
&F_6(\cdots\cdots)=-q_{31}-p_{32}+q_{43}-q_{24},\\
&F_7(\cdots\cdots)=q_{21}-p_{22}+q_{13}+q_{34},\\
&F_8(\cdots\cdots)=q_{11}+p_{12}-p_{23}+q_{44},\\
&\alpha_i=du_i-p_{i1}dx_1-p_{i2}dx_2-p_{i3}dx_3-p_{i4}dx_4\quad(i=1,\ldots,4),\\
&\beta_i=dv_i-q_{i1}dx_1-q_{i2}dx_2-q_{i3}dx_3-q_{i4}dx_4\quad(i=1,\ldots,4),
\end{aligned} \tag{2.6}$$

and $dF_1,\ldots,dF_8,d\alpha_1,\ldots,d\beta_4$.

For investigating the symmetries we consider the following vector fields (infinitesimal generators):

$$Z_1=\sum_{k=1}^{4}\left(u_k\frac{\partial}{\partial u_k}+v_k\frac{\partial}{\partial v_k}\right),$$

$$Z_2=\sum_{k=1}^{4}\left(u_k\frac{\partial}{\partial v_k}-v_k\frac{\partial}{\partial u_k}\right),$$

$$Z_3=u_1\frac{\partial}{\partial u_2}-u_2\frac{\partial}{\partial u_1}-u_3\frac{\partial}{\partial u_4}+u_4\frac{\partial}{\partial u_3}-v_1\frac{\partial}{\partial v_2}+v_2\frac{\partial}{\partial v_1}+v_3\frac{\partial}{\partial v_4}-v_4\frac{\partial}{\partial v_3},$$

$$Z_4=u_1\frac{\partial}{\partial v_2}-v_2\frac{\partial}{\partial u_1}+v_1\frac{\partial}{\partial u_2}-u_2\frac{\partial}{\partial v_1}-u_3\frac{\partial}{\partial v_4}+v_4\frac{\partial}{\partial u_3}-v_3\frac{\partial}{\partial u_4}+u_4\frac{\partial}{\partial v_3},$$

$$Z_5=u_1\frac{\partial}{\partial u_4}+u_4\frac{\partial}{\partial u_1}-u_2\frac{\partial}{\partial u_3}-u_3\frac{\partial}{\partial u_2}-v_1\frac{\partial}{\partial v_4}-v_4\frac{\partial}{\partial v_1}+v_2\frac{\partial}{\partial v_3}+v_3\frac{\partial}{\partial v_2},$$

$$Z_6=u_1\frac{\partial}{\partial v_4}+v_4\frac{\partial}{\partial u_1}+v_1\frac{\partial}{\partial u_4}+u_4\frac{\partial}{\partial v_1}-u_2\frac{\partial}{\partial v_3}-v_3\frac{\partial}{\partial u_2}-v_2\frac{\partial}{\partial u_3}-u_3\frac{\partial}{\partial v_2},$$

$$Z_7=u_1\frac{\partial}{\partial u_3}+u_3\frac{\partial}{\partial u_1}+v_1\frac{\partial}{\partial v_3}+v_3\frac{\partial}{\partial v_1}+u_2\frac{\partial}{\partial u_4}+u_4\frac{\partial}{\partial u_2}+v_2\frac{\partial}{\partial v_4}+v_4\frac{\partial}{\partial v_2},$$

$$Z_8=u_1\frac{\partial}{\partial v_3}-v_3\frac{\partial}{\partial u_1}+u_2\frac{\partial}{\partial v_4}-v_4\frac{\partial}{\partial u_2}+u_3\frac{\partial}{\partial v_1}-v_1\frac{\partial}{\partial u_3}+u_4\frac{\partial}{\partial v_2}-v_2\frac{\partial}{\partial u_4}, \tag{2.7}$$

The following theorems can easily be obtained by calculating the Lie bracket of the vector fields Z_i $(i=1,\ldots,8)$.

Theorem 1: The vector fields $Z_1,\ldots,Z_8$ form a basis of a nonabelian Lie algebra under the Lie bracket. The center is given by $\{Z_1, Z_8, 0\}$.

Theorem 2: The vector fields Z_1, Z_2, Z_5, Z_6 form a basis of a nonabelian Lie algebra under the Lie bracket.

Consider now the quantity $\psi^\dagger\psi$ and the vector fields $Z_1,\ldots,Z_8$. $\psi^\dagger\psi$ is a real quantity, i.e.,

$$\psi^\dagger\psi\equiv\sum_{j=1}^{4}(u_j^2+v_j^2). \tag{2.8}$$

Let $L_V(\cdot)$ denote the Lie derivative of a differential form with respect to a vector field V.

Theorem 3: The quantity $\psi^\dagger\psi$ is invariant under the vector fields Z_2, Z_3, Z_4, Z_8.

Proof: A straightforward calculation shows that

$$L_{Z_i}\psi^\dagger\psi=0\quad(i=2,3,4,8). \tag{2.9}$$

Theorem 4: The vector fields Z_2, Z_3, Z_4, Z_8 form a basis of a nonabelian Lie algebra under the Lie bracket.

The once-extended vector fields[2] of $Z_1,\ldots,Z_8$ are given by (compare Appendix)

$$\bar{Z}_1=Z_1+\sum_{j=1}^{4}\sum_{k=1}^{4}\left(p_{kj}\frac{\partial}{\partial p_{kj}}+q_{kj}\frac{\partial}{\partial q_{kj}}\right),$$

$$\bar{Z}_2=Z_2+\sum_{j=1}^{4}\sum_{k=1}^{4}\left(p_{kj}\frac{\partial}{\partial q_{kj}}-q_{kj}\frac{\partial}{\partial p_{kj}}\right),$$

$$\bar{Z}_3=Z_3+\sum_{j=1}^{4}\left[\left(p_{1j}\frac{\partial}{p_{2j}}-p_{2j}\frac{\partial}{p_{1j}}\right)+\left(-p_{3j}\frac{\partial}{\partial p_{4j}}+p_{4j}\frac{\partial}{\partial p_{3j}}\right)+\left(-q_{1j}\frac{\partial}{\partial q_{2j}}+q_{2j}\frac{\partial}{\partial q_{1j}}\right)+\left(q_{3j}\frac{\partial}{\partial q_{4j}}-q_{4j}\frac{\partial}{\partial q_{3j}}\right)\right],$$

$$\bar{Z}_4=Z_4+\sum_{j=1}^{4}\left[\left(p_{1j}\frac{\partial}{\partial q_{2j}}-q_{2j}\frac{\partial}{\partial p_{1j}}\right)+\left(q_{1j}\frac{\partial}{\partial p_{2j}}-p_{2j}\frac{\partial}{\partial q_{1j}}\right)+\left(-p_{3j}\frac{\partial}{\partial q_{4j}}+q_{4j}\frac{\partial}{\partial p_{3j}}\right)+\left(-q_{3j}\frac{\partial}{\partial p_{4j}}+p_{4j}\frac{\partial}{\partial q_{3j}}\right)\right],$$

$$\bar{Z}_5=Z_5+\sum_{j=1}^{4}\left[\left(p_{1j}\frac{\partial}{\partial p_{4j}}+p_{4j}\frac{\partial}{\partial p_{1j}}\right)+\left(-p_{2j}\frac{\partial}{\partial p_{3j}}-p_{3j}\frac{\partial}{\partial p_{2j}}\right)+\left(-q_{1j}\frac{\partial}{\partial q_{4j}}-q_{4j}\frac{\partial}{\partial q_{1j}}\right)+\left(q_{2j}\frac{\partial}{\partial q_{3j}}+q_{3j}\frac{\partial}{\partial q_{2j}}\right)\right],$$

$$\bar{Z}_6=Z_6+\sum_{j=1}^{4}\left[\left(p_{1j}\frac{\partial}{\partial q_{4j}}+q_{4j}\frac{\partial}{\partial p_{1j}}\right)+\left(q_{1j}\frac{\partial}{\partial p_{4j}}+p_{4j}\frac{\partial}{\partial q_{1j}}\right)+\left(-p_{2j}\frac{\partial}{\partial q_{3j}}-q_{3j}\frac{\partial}{\partial p_{2j}}\right)+\left(-q_{2j}\frac{\partial}{\partial p_{3j}}-p_{3j}\frac{\partial}{\partial q_{2j}}\right)\right],$$

$$\bar{Z}_7=Z_7+\sum_{j=1}^{4}\left[\left(p_{1j}\frac{\partial}{\partial p_{3j}}+p_{3j}\frac{\partial}{\partial p_{1j}}\right)+\left(q_{1j}\frac{\partial}{\partial q_{3j}}+q_{3j}\frac{\partial}{\partial q_{1j}}\right)+\left(p_{2j}\frac{\partial}{\partial p_{4j}}+p_{4j}\frac{\partial}{\partial p_{2j}}\right)+\left(q_{2j}\frac{\partial}{\partial q_{4j}}+q_{4j}\frac{\partial}{\partial q_{2j}}\right)\right],$$

$$\bar{Z}_8=Z_8+\sum_{j=1}^{4}\left[\left(p_{1j}\frac{\partial}{\partial q_{3j}}-q_{3j}\frac{\partial}{\partial p_{1j}}\right)+\left(p_{2j}\frac{\partial}{\partial q_{4j}}-q_{4j}\frac{\partial}{\partial p_{2j}}\right)+\left(p_{3j}\frac{\partial}{\partial q_{1j}}-q_{1j}\frac{\partial}{\partial p_{3j}}\right)+\left(p_{4j}\frac{\partial}{\partial q_{2j}}-q_{2j}\frac{\partial}{\partial p_{4j}}\right)\right]. \tag{2.10}$$

Calculating the Lie derivative of the differential forms given by Eq. (2.6) with respect to the vector fields given by Eq. (2.10), we find that the Lie derivatives are always elements of the differential ideal generated by the set $\{F_1,\ldots,F_8,\alpha_1,\ldots,\alpha_4,\beta_1,\ldots,\beta_4\}$. Consequently, the Dirac equation without rest mass is invariant under the infinitesimal generators $Z_1,\ldots,Z_8$. The transformation groups associated with the infinitesimal generators $Z_1,\ldots,Z_8$ are given by the Lie series

$$(u_1,\ldots,v_4)^{\mathrm{T}}\to\exp(\epsilon Z_i)(u_1,\ldots,v_4)^{\mathrm{T}}. \tag{2.11}$$

The space under consideration is $\mathbb{R}^8$. Since the autonomous system of differential equations associated with the vector fields $Z_1,\ldots,Z_8$ are linear it follows that the vector fields are complete. For example, Z_2 is associated with the transformation group ("duality rotation")

$$\begin{pmatrix}u_i\\ v_i\end{pmatrix}\to\begin{pmatrix}\cos\epsilon & -\sin\epsilon\\ \sin\epsilon & \cos\epsilon\end{pmatrix}\begin{pmatrix}u_i\\ v_i\end{pmatrix}, \tag{2.12}$$

where $i=1,\ldots,4$.

There are two points to be made.

Point 1: In order to obtain the linear symmetry generators $\bar{Z}_1,\ldots,\bar{Z}_8$ we make the general Ansatz

$$Z=\sum_{i,j=1}^{4}\left(a_{ij}u_i\frac{\partial}{\partial u_j}+b_{ij}v_i\frac{\partial}{\partial v_j}+c_{ij}v_i\frac{\partial}{\partial u_j}+d_{ij}u_i\frac{\partial}{\partial v_j}\right). \tag{2.13}$$

where $a_{ij}, b_{ij}, c_{ij}, d_{ij}\in\mathbb{R}$. Then we calculate the once-extended vector field $\bar{Z}$ (compare Appendix). To obtain the linear symmetry generators we require that

$$\begin{aligned}&L_{\bar{Z}}F_i\in\langle F_1,\ldots,F_8\rangle,\\ &L_{\bar{Z}}\alpha_i\in\langle F_1,\ldots,\beta_4\rangle,\end{aligned} \tag{2.14}$$

and so on, where $\langle\cdots\rangle$ denotes the differential ideal generated by $\{\cdots\}$. The coefficients $a_{ij},\ldots,d_{ij}$ are determined by the Eqs. (2.14). Equations (2.14) can be solved and we obtain the vector fields $\bar{Z}_1,\ldots,\bar{Z}_8$.

Point 2: We mention that the symmetry generators $Z_1,\ldots,Z_8$ can also be obtained by applying an approach described by Harrison and Estabrook.[5] They discussed briefly the massless Dirac equation written as a set of eight 3-forms in the field variables.

Consider now infinitesimal generators which are associated with the Lie-Bäcklund tangent transformation groups. We consider the vector fields

$$V^{(ij)} = F_i(p_{11}, \ldots, q_{44})\frac{\partial}{\partial u_j},$$
$$W^{(ij)} = F_i(p_{11}, \ldots, q_{44})\frac{\partial}{\partial v_j}, \tag{2.15}$$

where $i = 1, \ldots, 8$ and $j = 1, \ldots, 4$. $F_1(p_{11}, \ldots, q_{44}), \ldots, F_8(p_{11}, \ldots, q_{44})$ are given by Eq. (2.6). The calculation of the Lie derivatives of the differential forms $F_1, \ldots, F_8, \alpha_1, \ldots, \beta_4$ with respect to the vector fields $V^{(ij)}$ and $W^{(ij)}$ tells us that the vector fields $V^{(ij)}$ and $W^{(ij)}$ are infinitesimal generators which leave invariant the Dirac equation without rest mass. The Lie Bäcklund tangent transformation groups can be obtained by infinite extension of the infinitesimal generators. Finally, we notice that the commutators $[V^{(ij)}, Z_k]$ and $[W^{(ij)}, Z_k]$ are elements of a vector space V, where $k = 1, \ldots, 8$ and V is the vector space with the basis $\{V^{(ij)}, W^{(ij)}\}$.

3. DIRAC EQUATION WITH NONVANISHING REST MASS

Consider now the Dirac equation with rest mass m_0 written as

$$\sum_{k=1}^{3} \hbar \frac{\partial}{\partial x_k}(\gamma_k\psi) - i\hbar\frac{\partial}{\partial x_k}(\gamma_4\psi) + m_0 c\psi = 0. \tag{3.1}$$

Introducing the dimensionless quantity

$$\bar{x}_k \equiv m_0 c x_k/\hbar, \quad (k = 1, 2, 3, 4), \tag{3.2}$$

we obtain

$$\sum_{k=1}^{3} \frac{\partial}{\partial \bar{x}_k}(\gamma_k\psi) - i\frac{\partial}{\partial \bar{x}_4}(\gamma_k\psi) + \psi = 0. \tag{3.3}$$

In the following the bar is omitted. Again we put $\psi_k(x) = u_k(x) + iv_k(x)$ and find as above a linear system of eight coupled partial differential equations. In contrast to the Eq. (2.4) now not only the derivatives of the fields $u_k(x)$ and $v_k(x)$ occur, but also the fields $u_k(x)$ and $v_k(x)$. Thus we must study the following differential forms:

$$\begin{aligned}
F_1(u_1, \ldots, v_4, p_{11}, \ldots, q_{44}) &= -p_{41} - q_{42} - p_{33} - p_{14} + v_1,\\
F_2(\cdots\cdots\cdots) &= -p_{31} + q_{32} + p_{43} - p_{24} + v_2,\\
F_3(\cdots\cdots\cdots) &= p_{21} + q_{22} + p_{13} + p_{34} + v_3,\\
F_4(\cdots\cdots\cdots) &= p_{11} - q_{12} - p_{23} + p_{44} + v_4,\\
F_5(\cdots\cdots\cdots) &= -q_{41} + p_{42} - q_{33} - q_{14} - u_1,\\
F_6(\cdots\cdots\cdots) &= -q_{31} - p_{32} + q_{43} - q_{24} - u_2,\\
F_7(\cdots\cdots\cdots) &= q_{21} - p_{22} + q_{13} + q_{34} - u_3,\\
F_8(\cdots\cdots\cdots) &= q_{11} + p_{12} - q_{23} + q_{44} - u_4,
\end{aligned} \tag{3.4}$$

$\alpha_1, \ldots, \beta_4$.

$\alpha_1, \ldots, \beta_4$ are given by Eq. (2.6). We may well ask which vector fields given by Eq. (2.7) and (2.10) leave invariant the differential forms written above. By calculating the Lie derivatives of the differential forms given above with respect to the vector fields $\bar{Z}_1, \ldots, \bar{Z}_8$, we find that the Dirac equation with rest mass m_0 is invariant under the vector fields Z_1, Z_2, Z_5, Z_6. Again infinitesimal generators which are associated with Lie Bäcklund tangent transformation groups can be given at once, namely

$$V^{(ij)} = F_i(u_1, \ldots, q_{44})\partial/\partial u_j,$$
$$W^{(ij)} = F_i(u_1, \ldots, q_{44})\partial/\partial v_j, \tag{3.5}$$

where $i = 1, \ldots, 8$ and $j = 1, \ldots, 4$. $F_1(u_1, \ldots, q_{44}), \ldots, F_8(u_1, \ldots, q_{44})$ are given by Eq. (3.4). The calculation of the Lie derivatives of the differential forms $F_1, \ldots, F_8, \alpha_1, \ldots, \beta_4$ with respect to the vector fields $V^{(ij)}$ and $W^{(ij)}$ shows that the vector fields $V^{(ij)}$ and $W^{(ij)}$ are infinitesimal generators which leave invariant the Dirac equation with rest mass.

4. NONLINEAR DIRAC EQUATION

Let us study the infinitesimal symmetries of the Dirac equation with a nonlinear term. We add the nonlinear term $\psi(\bar{\psi}\psi)$ to the left-hand side of Eq. (3.3). Then we obtain the nonlinear Dirac equation

$$\sum_{k=1}^{3} \frac{\partial}{\partial \bar{x}_k}(\gamma_k\psi) - i\frac{\partial}{\partial \bar{x}_4}(\gamma_4\psi) + \psi + \psi(\bar{\psi}\psi) = 0, \tag{4.1}$$

where $\bar{\psi} = (\psi_1^*, \psi_2^*, -\psi_3^*, -\psi_4^*)$. Again let us put $\psi_k(x) = u_k(x) + iv_k(x)$. We then have a coupled system of eight nonlinear partial differential equations.

Now we should ask whether the nonlinear Dirac equation obtained in this way is invariant under the vector fields given by Eq. (2.10). A straightforward calculation (again we have to calculate the Lie derivative) leads to the following theorem:

Theorem 5: The nonlinear Dirac equation given by Eq. (4.1) is invariant under Z_2.

APPENDIX

In order to consider the infinitesimal symmetries, we need the once-extended vector field.[1] Let

$$V = \sum_{j}^{n} \xi_j(x, \phi)\frac{\partial}{\partial x_j} + \sum_{i=1}^{m} \eta_i(x, \phi)\frac{\partial}{\partial \phi_i}.$$

Then the once-extended vector field is given by $(\partial\phi_i/\partial x_j \to p_{ij})$,

$$\bar{V} = V + \sum_{j=1}^{n}\sum_{i=1}^{m}\left[\frac{\partial \eta_i}{\partial x_j} + \sum_{k=1}^{m}\frac{\partial\eta_i}{\partial\phi_k}p_{kj} - \sum_{k=1}^{n}\frac{\partial\xi_k}{\partial x_j}p_{ik} - \sum_{k=1}^{n}\sum_{l=1}^{m}\frac{\partial\xi_k}{\partial\phi_l}p_{lj}p_{ik}\right]\frac{\partial}{\partial p_{ij}}.$$

Consider an important special case. Let

$$W = \sum_{i=1}^{8}\eta_i(\phi)\frac{\partial}{\partial\phi_i}.$$

Then, a special case, we have $(n = 4, m = 8)$

$$\bar{W} = W + \sum_{j=1}^{4}\sum_{i=1}^{8}\left(\sum_{k=1}^{8}\frac{\partial\eta_i}{\partial\phi_k}p_{kj}\right)\frac{\partial}{\partial p_{ij}}.$$

For the present case, we have $\phi_i \equiv u_i$ ($i=1,2,3,4$), $\phi_i \equiv v_i$ ($i=5,6,7,8$), and $p_{4+ij} = q_{ij}$ ($i=1,2,3,4$). Let

$$X = \phi_k \frac{\partial}{\partial \phi_i}.$$

Then

$$\bar{X} = X + \sum_{j=1}^{4} p_{kj} \frac{\partial}{\partial p_{ij}}.$$

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Some spectral properties in algebras of unbounded operators [a)]

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Some aspects of spectral theory in algebras of unbounded operators are studied. After having pointed out the pathologies of the spectral behavior of these operators we give a sufficient condition in order that a self-adjoint operator admit a spectral decomposition with spectral measure with values in the same algebra. Some examples illustrating the developed ideas are given.

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1. INTRODUCTION

In recent years many authors have devoted their attention to the study of algebras of unbounded operators, both from the mathematical point of view and for applications in quantum physics [see, for instance Refs. 1–6; we indicate it with the symbol $C_{\mathfrak{D}}$ and other authors with the symbol $L^{\dagger}(\mathfrak{D})$].

This algebra, which consists of the class of operators everywhere defined in a pre-Hilbert space $\mathfrak{D}$, having everywhere defined adjoints [equivalently, continuous with respect to the weak topology induced by the maps $\varphi \to (\varphi, \psi), \psi \in \mathfrak{D}$], shows some analogy with the well-known algebra $B(\mathfrak{H})$ of all bounded operators in Hilbert space $\mathfrak{H}$, to which $C_{\mathfrak{D}}$ reduces when $\mathfrak{D}$ is chosen to be complete. For instance, it has been proved that a matrix representation for the operators of $C_{\mathfrak{D}}$ can be made, in strict analogy to what holds true for bounded operators in Hilbert space.[7,8]

The algebra $C_{\mathfrak{D}}$ seemed to be the best candidate for unbounded representations of algebras which cannot be represented with bounded operators (for an example see Ref. 9, Sec. 6, Theorem). The theory of unbounded representation of *-algebras has been the subject of many interesting papers (see, for instance, Refs. 6 and 10) in view of its applications in quantum field theory and in theory of Lie algebras.

Our problem is to see if it is possible to find other analogies between $C_{\mathfrak{D}}$ and $B(\mathfrak{H})$. In this paper, we examine, in particular, the spectral behavior of self-adjoint elements of $C_{\mathfrak{D}}$, that is we investigate the possibility of doing a spectral decomposition of these operators, in the sense that the spectral family associated with them, when it exists, takes its values in the same algebra $C_{\mathfrak{D}}$ (in this case we say that the operator is "$\mathfrak{D}$-spectral").

This problem has a well-known solution when the operators are completely continuous (see, for example, Ref. 11 n. 93). This depends on the fact that the eigenmanifolds of a compact operator, being finite dimensional, are all orthocomplemented also in pre-Hilbert space. But for noncompact operators many pathologies arise as a consequence of the fact that not all closed subspaces of a pre-Hilbert space $\mathfrak{D}$ admit a projection operator in $\mathfrak{D}$ (see Ref. 12). Furthermore notice that, with a suitable definition of spectrum, the spectrum of a self-adjoint operator of $C_{\mathfrak{D}}$ may fail to be all real.

In this paper, after having introduced suitable topologies in the pre-Hilbert space $\mathfrak{D}$, we examine some properties of the spectrum of self-adjoint elements of $C_{\mathfrak{D}}$. Finally we give a sufficient condition for the "$\mathfrak{D}$-spectrality" of a self-adjoint operator of $C_{\mathfrak{D}}$; this condition is automatically satisfied in $B(\mathfrak{H})$.

We illustrate the developed ideas by means of some examples.

2. NOTATION AND PRELIMINARY DEFINITIONS

Let $\mathfrak{D}$ be a scalar product space. We will denote with $C_{\mathfrak{D}}$ the *-algebra of all linear operators in $\mathfrak{D}$ which have an adjoint in $\mathfrak{D}$; or, equivalently, the *-algebra of all $\sigma(\mathfrak{D},\mathfrak{D})$-continuous operators. The $\sigma(\mathfrak{D},\mathfrak{D})$-topology is understood to be that defined by the set of seminorms

$$\{\varphi \to |(\varphi, \psi)| / \psi \in \mathfrak{D}\}.$$

We will denote with $B_{\mathfrak{D}}$ the subalgebra of all bounded operators of $C_{\mathfrak{D}}$.

We will denote with $\mathfrak{H}$ the Hilbert space which is the completion of $\mathfrak{D}$ in the norm-topology, defined in the usual way by the scalar product.

Then $C_{\mathfrak{D}}$ can be understood to be the set of all closable operators A in $\mathfrak{H}$ having $\mathfrak{D}$ as a dense common invariant domain and such that $A^*(\mathfrak{D}) \subseteq \mathfrak{D}$. The involution in $C_{\mathfrak{D}}$ is then defined by $A \to A^{+}$ with $A^{+} = A^*/\mathfrak{D}$.

If S is an operator in $\mathfrak{H}$ with $D(S)$ we indicate its domain and with $\overline{S}$ its closure in $\mathfrak{H}$

With $\mathscr{A} \subseteq C_{\mathfrak{D}}$ we will mean that $\mathscr{A}$ is an involutive subalgebra, with unity, of $C_{\mathfrak{D}}$. (Some authors say, in this case, that $\mathscr{A}$ is an op*-algebra.)

If $\mathscr{B} \subseteq C_{\mathfrak{D}}$, we will indicate with $\mathscr{B}'$ the weak commutant of $\mathscr{B}$, i.e., the set

$$\mathscr{B}' = \{B \in B(\mathfrak{H}) : (S^{+}\varphi, B\psi) = (\varphi, BS\psi) \quad \forall \varphi, \psi \in \mathfrak{D} \quad \forall S \in \mathscr{B}\}.$$

The commutants of higher order are defined in the usual way in $B(\mathfrak{H})$; for instance,

$$\mathscr{B}'' = \{C \in B(\mathfrak{H}) : BC = CB, \quad \forall B \in \mathscr{B}'\}.$$

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If $\mathscr{B}\subseteq C_{\mathfrak{D}}$, with the notation $[\mathscr{B}]$ we mean the subalgebra of $C_{\mathfrak{D}}$ generated by $\mathscr{B}$. When $\mathscr{B}=\{A\}$ we will write $[A]$ instead of $[\{A\}]$.

3. $\mathscr{A}$-TOPOLOGIES, RESOLVENT, AND SPECTRUM

Definition 1: Let $\mathscr{A}\leqslant C_{\mathfrak{D}}$. We say that $\mathfrak{D}$ is endowed with the $\mathscr{A}$-topology, if the topology in $\mathfrak{D}$ is defined by the set of seminorms

$$\{\varphi\to\|A\varphi\|/A\in\mathscr{A}\}.$$

Remark: The fact that $I\in\mathscr{A}$ implies that the $\mathscr{A}$-topology is, generally, finer than the norm topology.

If every operator $A\in\mathscr{A}$ is bounded then the $\mathscr{A}$-topology coincides with the norm topology. Particularly, if $\mathfrak{D}$ is complete under the norm topology, we have $C_{\mathfrak{D}}=B(\mathfrak{H})$ and then all $\mathscr{A}$-topologies coincide with the norm topology.

Definition 2: Let $\mathscr{A}\leqslant C_{\mathfrak{D}}$. Let

$$\mathfrak{D}^*=\bigcap_{A\in\mathscr{A}}D(A^*).$$

We say that $\mathfrak{D}$ is $\mathscr{A}$-self-adjoint if $\mathfrak{D}^*=\mathfrak{D}$.

Proposition 3: If $\mathscr{A}\leqslant C_{\mathfrak{D}}$, the following propositions are equivalent:

(i) $\mathfrak{D}$ is complete under the $\mathscr{A}$-topology.

(ii) $\mathfrak{D}=\bigcap_{A\in\mathscr{A}}D(\bar{A})$

Proof: It follows from Ref. 10, Theorem 1, n. 4, and from the fact that $\mathscr{A}$, being an op*-algebra, is directed, that is, $\forall A_1,A_2\in\mathscr{A}$ there is $A_3\in\mathscr{A}$ such that $\max\{\|A_1\varphi\|,\|A_2\varphi\|\}\leqslant\|A_3\varphi\|$, $\forall\varphi\in\mathscr{D}$. See, also Ref. 3 Lemma 3.2.

We will now prove the following:

Proposition 4: Let $\mathscr{A}\leqslant C_{\mathfrak{D}}$. If $\mathfrak{D}$ is $\mathscr{A}$-self-adjoint, then $\mathfrak{D}$ is complete under the $\mathscr{A}$-topology.

Proof: We have, in fact

$$\mathfrak{D}\subseteq\bigcap_{A\in\mathscr{A}}D(\bar{A})=\bigcap_{A\in\mathscr{A}}D(\bar{A}^+)\subseteq\bigcap_{A\in\mathscr{A}}D(A^*)=\mathfrak{D}^*=\mathfrak{D}.$$

The statement follows from Proposition 3.

Because of the fact that $C_{\mathfrak{D}}$ is an algebra it should be very natural to give the definition of resolvent set of an element $T\in C_{\mathfrak{D}}$ in the usual algebraic way. But, as Schaefer in Ref. 13 has pointed out, this definition, in a locally convex algebra, is of little use, in contrast with what happends for Banach algebras. Also in our case, the algebraic definition does not allow us to obtain for the resolvent set (and hence for the spectrum) of an operator of $C_{\mathfrak{D}}$ properties analogous to those which hold true for an element of the algebra $B(\mathfrak{H})$ of all bounded operators in Hilbert space $\mathfrak{H}$. We will then give the following definition.

Definition 5: Let $T\in C_{\mathfrak{D}}$, we call resolvent set of T the subset of the complex field **C**

$$\rho(T)=\{\lambda\in\mathbf{C}:\ \text{there exists}\quad (T-\lambda I)^{-1}\in B_{\mathfrak{D}}\}.$$

As usual, we call spectrum of T the set $\sigma(T)=\mathbf{C}-\rho(T)$.

Remark: If $\mathfrak{D}$ is complete in the norm topology, then the above definition coincides with the algebraic one, as it is easy to see.

The resolvent set (and hence the spectrum) of an operator of $C_{\mathfrak{D}}$ has a behavior very different from that of an operator of $B(\mathfrak{H})$. For instance, the spectrum of a self-adjoint element of $C_{\mathfrak{D}}$ may fail to be real (i.e., $\sigma(T)\not\subseteq\mathbf{R}$) whereas, as it is easy to see, eigenvalues (if they exist) are all real. We consider, in fact, the following example.

Let $\mathfrak{D}=\{f\in L^2(\mathbf{R}):f(x)=p(x)\exp(-x^2/2), p(x)$ polynomial$\}$ and let T be the operator defined by

$$T:f(x)\in\mathfrak{D}\to xf(x)\in\mathfrak{D}.$$

If $\lambda\in\mathbf{C}$, the operator $T-\lambda I$ is defined by

$$(T-\lambda I)f(x)=(x-\lambda)f(x).$$

This operator, $\forall\lambda\in\mathbf{C}$, is not "onto" in $\mathfrak{D}$. Indeed, if we suppose that it be, then any polynomial over the complex field could be written in the form

$$p(x)=(x-\lambda)q(x),$$

with $q(x)$ a suitable polynomial. This is not obviously true. Then, in such a case, $\rho(T)=\phi$ and $\sigma(T)=\mathbf{C}$.

Definition 6: Let $T\in C_{\mathfrak{D}}$, we call resolvent function R_λ of T the map of **C** in the set of linear operators in $\mathfrak{D}$ defined by

$$R_\lambda=(T-\lambda I)^{-1}$$

whenever this inverse exists. In general, the resolvent set $\rho(T)$ of T is a proper subset of the domain of the function R_λ.

For completeness we report some proposition which can be easily proved.

Proposition 7: Let $T\in C_{\mathfrak{D}}$, $\rho(T)$ its resolvent set and R_λ its resolvent function. We have

(i) If $\lambda\in\rho(T)$ then $\bar{\lambda}\in\rho(T^+)$ and then $\rho(T^+)=\overline{\rho(T)}$.

(ii) $\forall\lambda,\mu\in\rho(T)$ we have (Hilbert relation)

$$R_\lambda-R_\mu=(\lambda-\mu)R_\lambda R_\mu.$$

(iii) $\forall\lambda,\mu\in\rho(T)$

$$R_\lambda R_\mu=R_\mu R_\lambda.$$

(iv) If $T=T^+$ all eigenvalues are real.

(v) If $T=T^+$, the number λ is an eigenvalue of T if, and only if the $\sigma(\mathfrak{D},\mathfrak{D})$-closure of the range $\Delta_T(\lambda)$ of the operator $T-\lambda I$ is different from $\mathfrak{D}$ i.e.,

$$\overline{\Delta_T(\lambda)}^w\neq\mathfrak{D}$$

If we assume that $\mathfrak{D}$ be complete in a suitable $\mathscr{A}$-topology, it is possible to find properties of the spectrum of an operator of $C_{\mathfrak{D}}$ analogous to those which hold true for the spectrum of a bounded operator in Hilbert space.

Theorem 8: Let $T\in C_{\mathfrak{D}}$. If there is an algebra $\mathscr{A}\leqslant C_{\mathfrak{D}}$ such that $\mathfrak{D}$ is complete in the $\mathscr{A}$-topology and $[T]''\subseteq\mathscr{A}'$, then the spectrum $\sigma(T)$ of the operator T is closed.

Proof: We will show that $\rho(T)$ is open. For $\lambda_0\in\rho(T)$ we have

$$\|(T-\lambda_0 I)\varphi\|\geqslant\|R_{\lambda_0}\|^{-1}\|\varphi\|,\quad\forall\varphi\in\mathfrak{D}.$$

For δ such that $0 < \delta < \epsilon^{-1}\|R_{\lambda_0}\|^{-1}$ with $\epsilon > 1$, we have for $|\lambda_0 - \lambda| < \delta$ and $\varphi \in \mathfrak{D}$

$$\|(T-\lambda I)\varphi\| \geq \|(T-\lambda_0 I)\varphi\| - \delta\|\varphi\| \geq (1-\epsilon^{-1})\|R_{\lambda_0}\|^{-1}\|\varphi\|.$$

Then λ is not an eigenvalue of T and the operator $T-\lambda I$ has a bounded inverse. It remains for us to prove that this inverse is everywhere defined and invariant in $\mathfrak{D}$ or, equivalently that $\forall\psi\in\mathfrak{D}$ there is, in $\mathfrak{D}$, a solution of the equation

$$(T-\lambda I)\varphi = \psi.$$

Letting $\varphi_n = \sum_{k=1}^n (\lambda-\lambda_0)^{k-1}R_{\lambda_0}^k\psi$, we prove that $\{\varphi_n\}$ is a Cauchy sequence in the $\mathscr{A}$-topology. In fact, if $A\in\mathscr{A}$, from $R_\lambda^k \in [T]'' \subseteq \mathscr{A}'$ $k\in N$, it follows that

$$\begin{aligned}\|A(\varphi_n-\varphi_m)\| &= \|A\sum_{k=m+1}^n (\lambda-\lambda_0)^{k-1}R_{\lambda_0}^k\psi\| \\ &= \|\sum_{k=m+1}^n (\lambda-\lambda_0)^{k-1}R_{\lambda_0}^k A\psi\| \\ &\leq \sum_{k=m+1}^n |\lambda-\lambda_0|^{k-1}\|R_{\lambda_0}^k\|\|A\psi\| \leq \|A\psi\|\|R_{\lambda_0}\| \\ &\times \sum_{k=m+1}^n \epsilon^{1-k} \to 0 \quad \text{when} \quad m,n\to\infty.\end{aligned}$$

For the completeness of $\mathfrak{D}$ in the $\mathscr{A}$-topology, there exists $\varphi\in\mathfrak{D}$ such that

$$\varphi = \sum_{n=1}^{\infty} (\lambda-\lambda_0)^{n-1}R_{\lambda_0}^n\psi. \tag{1}$$

Finally, we show that $\varphi = R_\lambda\psi$. From (1), which holds true, also in the $\sigma(\mathfrak{D},\mathfrak{D})$-topology, with respect to which $T-\lambda I$ is continuous, we have

$$(T-\lambda I)\varphi = (T-\lambda_0 I)\varphi - (\lambda-\lambda_0)\varphi = \sum_{n=1}^{\infty}(\lambda-\lambda_0)^{n-1}R_{\lambda_0}^{n-1} - \sum_{n=1}^{\infty}(\lambda-\lambda_0)^n R_{\lambda_0}^n\psi = \psi.$$

The statement is proved.

In the proof of the above theorem we have, implicitly, shown that

Corollary 9: In the hypothesis of preceding theorem, for every $\lambda_0\in\rho(T)$ the function $\lambda\to R_\lambda\psi$ admits the following development in power series

$$R_\lambda\psi = R_{\lambda_0}\psi + (\lambda-\lambda_0)R_{\lambda_0}^2\psi + (\lambda-\lambda_0)^2R_{\lambda_0}^3\psi + \cdots$$

for all λ such that $|\lambda-\lambda_0| < \|R_{\lambda_0}\|^{-1}$ and $\forall\psi\in\mathfrak{D}$.

4. SPECTRAL BEHAVIOR OF $\mathfrak{D}$-SELF-ADJOINT OPERATORS

In the sequel, an operator $T\in C_{\mathfrak{D}}$ is said to be $\mathfrak{D}$-self-adjoint if $T = T^\dagger$.

Definition 10: Let T be a $\mathfrak{D}$-self-adjoint operator. We say that T is $\mathfrak{D}$-spectral

(i) if there is a unique self-adjoint extension $\hat{T}$ of T to $\mathfrak{H}$.

(ii) if $\{E_\lambda\}_{-\infty}^{+\infty}$ is the spectral family associated with $\hat{T}$ then

$$E_\lambda(\mathfrak{D})\in\mathfrak{D} \quad \forall\lambda\in\mathbf{R}.$$

We examine, first, the question of the existence of a self-adjoint extension of the operator T.

A $\mathfrak{D}$-self-adjoint operator T may be regarded as a symmetric operator in $\mathfrak{H}$ and the theory of the existence of self-adjoint extensions of symmetric operators in is well known (see, for instance, Ref. 11 n. 123) and it is also known that an essentially self-adjoint operator in $\mathfrak{H}$ has a unique self-adjoint extension (see Ref. 14, Sec. VIII. 2).

Let us give a sufficient condition in order that a $\mathfrak{D}$-self-adjoint operator of $C_{\mathfrak{D}}$ be essentially self-adjoint in $\mathfrak{H}$, this condition can be very useful in some cases.

Proposition 11: Let T be a $\mathfrak{D}$-self-adjoint operator. If the complex number i is an element of $\rho(T)$ then T is essentially self-adjoint in $\mathfrak{H}$.

Proof: The operator T is symmetric in $\mathfrak{H}$ and we know that a symmetric operator T defined in $\mathfrak{H}$ is essentially self-adjoint if and only if (see Ref. 14, Sec. VIII. 2, Corollary)

$$\operatorname{Ker}(T^* \pm iI) = \{0\}.$$

We suppose that $i\in\rho(T)$ and $\operatorname{Ker}(T^*\pm iI)\neq\{0\}$. But in this case there exists $\varphi\in\mathfrak{H}$ such that

$$T^*\varphi + i\varphi = 0,$$

then $-i$ is an eigenvalue of T^* and therefore $(T-iI)^{-1}$ does not belong to $B(\mathfrak{H})$ and consequently to $L_{\mathfrak{D}}$. This contrasts our hypothesis.

We now give the condition that an operator $T\in C_{\mathfrak{D}}$ be $\mathfrak{D}$-spectral.

Lemma 12: Let $\mathscr{A}\subset C_{\mathfrak{D}}$. If $\mathfrak{H}$ is $\mathscr{A}$-self-adjoint and S is an operator in $\mathfrak{H}$ such that $D(S)\supseteq\mathfrak{D}$ and $\forall A\in\mathscr{A}$

$$(A^\dagger\varphi, S\psi) = (\varphi, SA\psi) \quad \forall\varphi,\psi\in\mathfrak{D} \tag{2}$$

then $S(\mathfrak{D})\subseteq\mathfrak{D}$.

Proof: From (2), using Schwartz's inequality, it follows that

$$|(A^\dagger\varphi, S\psi)| \leq K\|\varphi\|, \quad \text{with} \quad K = \|SA\psi\|,$$

then $S\psi\in D((A^\dagger)^*)$ $\forall A\in\mathscr{A}$, i.e.:

$$S\psi\in \bigcap_{A\in\mathscr{A}} D((A^\dagger)^*) = \bigcap_{A\in\mathscr{A}} D(A^*) = \mathfrak{D}^* = \mathfrak{D}.$$

From the arbitrariness of $\psi\in\mathfrak{D}$, it follows $S(\mathfrak{D})\subseteq\mathfrak{D}$

Theorem 13: Let $T\in C_{\mathfrak{D}}$ be a $\mathfrak{D}$-self-adjoint operator, such that the following conditions be satisfied:

(a) T has a unique self-adjoint extension to $\mathfrak{H}$.

(b) There exists an algebra $\mathscr{A}\subset C_{\mathfrak{D}}$ such that $[T]''\subseteq\mathscr{A}'$, and $\mathfrak{D}$ be $\mathscr{A}$-self-adjoint.

Then T is a $\mathfrak{D}$-spectral operator.

Proof: We indicate with $\hat{T}$ the unique self-adjoint extension of T to $\mathfrak{H}$. Let $\{E_\lambda\}$ be the spectral family of $\hat{T}$ in $\mathfrak{H}$, that is

$$\hat{T}\varphi = \int_{-\infty}^{+\infty}\lambda\, dE_\lambda\varphi, \quad \forall\varphi\in D(\hat{T}).$$

We will prove that $E_\lambda\in[T]''$. Let $B\in[T]'$, then by definition of Sec. 1,

$$(T\varphi, B\psi) = (\varphi, BT\psi), \quad \forall \varphi, \psi \in \mathfrak{D}.$$

It follows easily that

$$((T - iI)^{-1}\varphi, B\psi) = (\varphi, B(T + iI)^{-1}\psi) \quad \forall \varphi, \psi \in \mathfrak{D}.$$

For the boundedness of the operators $(T \pm iI)^{-1}$, the above relation can be extended in all $\mathfrak{H}$ and then

$$B(\hat{T} + iI)^{-1} = (\hat{T} + iI)^{-1}B.$$

Hence B commutes also with $\hat{T} + iI$ and then with $\hat{T}$, i.e.,

$$B\hat{T} \subseteq \hat{T}B.$$

It follows that $E_\lambda \in [T]'' \subseteq \mathscr{A}'$.

Then

$$(A^+\varphi, E_\lambda\psi) = (\varphi, E_\lambda A\psi) \quad \forall A \in \mathscr{A}, \ \forall \varphi, \psi \in \mathfrak{D}.$$

By Lemma 12 it follows that

$$E_\lambda(\mathfrak{D}) \subseteq \mathfrak{D}, \quad \forall \lambda \in \mathbf{R}.$$

The conditions given in the above theorem are, clearly, very strong, but we can give some examples of operators of $C_{\mathfrak{D}}$ which are $\mathfrak{D}$-spectral (see Appendix).

Remark: All conditions given in Theorem 13 for the $\mathfrak{D}$-spectrality are automatically satisfied, if $\mathfrak{D}$ is complete and hence $C_{\mathfrak{D}} = B(\mathfrak{H})$, for a self-adjoint operator of $B(\mathfrak{H})$. In fact, in this case, for any subalgebra $\mathscr{A}$ of $B(\mathfrak{H})$, the $\mathscr{A}$-topology coincides with the usual norm-topology.

Theorem 14: Let T be a $\mathfrak{D}$-self-adjoint operator. Suppose that there is an algebra $\mathscr{A} \leq C$ such that $[T]'' \subseteq \mathscr{A}'$ and $\mathfrak{D}$ be $\mathscr{A}$-self-adjoint. Then, if T has a self-adjoint extension $\hat{T}$ to $\mathfrak{H}$, $\sigma(T) \subseteq \mathbf{R}$.

Proof: Let $\lambda \in \mathbf{C} - \mathbf{R}$, then the operator $(\hat{T} - \lambda I)^{-1} \in B(\mathfrak{H})$ exsists. We prove that it is invariant in $\mathfrak{D}$.

Let $B \in [T]'$. In an analogous way to that of Theorem 15, we can prove that

$$B\hat{T} \subseteq \hat{T}B$$

and hence $(\hat{T} - \lambda I)^{-1}$ commutes with B. Then $(\hat{T} - \lambda I)^{-1} \in [T]'' \subseteq \mathscr{A}'$.

The statement follows from Lemma 12.

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APPENDIX

Let us give some example of $\mathfrak{D}$-spectral operators of $C_{\mathfrak{D}}$.

Example 1: Let $\mathfrak{D} = \{f \in L^2(\mathbf{R}) : x^n f(x) \in L^2(\mathbf{R}) \ \forall n \in \mathbf{N}\}$.

It is easily seen that $\mathfrak{D}$ is a dense proper linear manifold of $L^2(\mathbf{R})$. Let T be the operator defined by

$$(Tf)(x) = xf(x), \quad \forall f \in \mathfrak{D}.$$

It is clear that T is $\mathfrak{D}$-self-adjoint.

With easy considerations can be stated that $\sigma(T) \subseteq \mathbf{R}$, because for any complex nonreal number λ the operator $(T - \lambda I)^{-1}$ is an element of $B_{\mathfrak{D}}$.

We choose $\mathscr{A} = [T]$. It is obvious that $\mathscr{A}'' \subseteq \mathscr{A}'$. We will prove that $\mathfrak{D}$ is $\mathscr{A}$-self-adjoint. We have

$$\mathfrak{D}^* = \bigcap_{A \in \mathscr{A}} D(A^*) = \bigcap_{n=1}^{\infty} D((T^n)^*).$$

But it is obvious that $\forall n \in \mathbf{N}$

$$D((T^n)^*) = \{f \in L^2(\mathbf{R}) : x^n f(x) \in L^2(\mathbf{R})\}.$$

And so $\mathfrak{D}^* = \mathfrak{D}$. Then for the operator T, Theorem 13 holds true.

It is well known, in fact, that the spectral family associated in $L^2(\mathbf{R})$, to the multiplication operator, is given by

$$(E_\lambda f)(x) = \chi_\lambda(x) f(x),$$

where $\chi_\lambda(x)$ is understood to be the characteristic function of the set $[-\infty, \lambda]$. It is easy to verify that $E_\lambda(\mathfrak{D}) \subseteq \mathfrak{D}$

Example 2: Let $\mathfrak{D}$ be the Schwartz's space $\mathscr{S}(\mathbf{R})$ of all complex infinitely differentiable functions such that

$$\lim_{|x| \to \infty} \left| x^k \frac{d^p}{dx^p} \varphi(x) \right| = 0, \ \forall k, p \geq 0.$$

Let $H = \frac{1}{2}(p^2 + q^2)$, where p and q are the operators defined, respectively, by

$$(p\psi)(x) = i\frac{d}{dx}\psi(x),$$

$$(q\psi)(x) = x\psi(x).$$

It is a known fact that $H^n/\mathscr{S}(\mathbf{R})$ is an essentially self-adjoint operator (for all $n \in \mathbf{N}$) and then it has a unique self-adjoint extension to $\mathfrak{H} = L^2(\mathbf{R})$.

We choose $\mathscr{A} = [H]$. It is easy to see that $\mathscr{A}'' \subseteq \mathscr{A}'$.

We will prove that $\mathfrak{D}$ is $\mathscr{A}$-self-adjoint. We have

$$\mathfrak{D}^* = \bigcap_{A \in \mathscr{A}} D(A^*) = \bigcap_{n=1}^{\infty} D((H^n)^*) = \bigcap_{n=1}^{\infty} D(\overline{H^n}) = \mathfrak{D}. \quad (3)$$

The last equality in (3) follows from the fact that $\varphi \in \mathscr{S}(\mathbf{R})$ if and only if $\varphi \in D(\overline{H^n})$, $\forall n \in \mathbf{N}$ (see Ref. 6, Sec. V, Example 2).

Then the operator H, by Theorem 13 is $\mathfrak{D}$-spectral.

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On Euler characteristics of compact Einstein 4-manifolds of metric signature $(+ + - -)$

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In the present paper, the Euler characteristic is studied for a compact oriented Einstein 4-manifold of signature $(+ + - -)$. For such a manifold, there are three types of normal forms of the curvature tensor. It is shown that for each type the Euler characteristic is nonnegative and even. Several new inequalities are obtained concerning the Euler characteristic and the volume of the manifold. The second Betti number is even, and if it is zero, then the first Betti number also vanishes. The arguments developed here are based upon the famous work of Chern about the Gauss–Bonnet formula for a pseudo-Riemannian manifold.

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I. INTRODUCTION

The characteristic classes of an Einstein 4-manifold are now the interesting objects from both mathematical and physical points of view. As to the compact oriented Einstein 4-manifold, the Euler characteristic is known to be nonnegative, and vanishes if and only if the manifold is flat.[1] Certain inequalities are known concerning the Euler characteristic and the Hirzebruch index.[2] A recent result is that, for the manifold of the positive sectional curvature, it is bounded above by a constant multiple of the squared scalar curvature.[3] Recently a few reports have been published about useful inequalities for Einstein Kähler manifolds[4,5] and conformally flat Einstein manifolds.[5] All the works stated above are concerned with the Einstein 4-manifolds of Reimannian metric.

Four-dimensional manifolds may possess one of three different metric signatures $(+ + + +)$, $(+ + + -)$, $(+ + - -)$. For a compact oriented manifold of dimension greater than two, it is known that the manifold admits a Lorentz metric if and only if the Euler characteristic vanishes.[6] Such a problem remains untreated for the last type of signature, to which we now focus our attention.

For pseudo-Riemannian manifolds, the generalized Gauss–Bonnet formula has been obtained by Chern.[7] The present paper is built upon the basis of the work of Chern and deals with the Euler characteristic of a compact oriented Einstein 4-manifold of metric signature $(+ + - -)$. Analogous to the works of Petrov[8,9] and Singer and Thorpe,[10] the normal (or canonical) forms for the curvature tensors are given. There are three types of normal forms which are quite similar to those of the Lorentz case. It is found that for a compact oriented Einstein 4-manifold the Euler characteristic is nonnegative and even. In Sec. II, the normal forms of the curvature tensors are treated. The main theorem and the results are stated in Sec. III.

II. NORMAL FORMS OF CURVATURES

By a manifold we mean a connected, paracompact, C^∞-differentiable manifold. Consider a 4-manifold of signature $(+ + - -)$. Let Λ^p denote the space of exterior p-forms on the manifold. The space Λ^p is endowed with an inner product $(\ ,\ )$ induced by the metric. Select a continuous field of orthonormal basis of 1-forms $\{e^i\}$ $(i = 1, ..., 4)$ with the inner product

$$(e^i,e^j) = \epsilon^i\delta^{ij}\ (\delta^{ij}\text{: Kronecker delta}) \tag{1}$$

with sign symbols $\epsilon^1 = \epsilon^2 = -\epsilon^3 = -\epsilon^4 = 1$.

The 2-forms are important since the curvature defines a linear transformation in Λ^2. A basis is given in terms of $\{e^i\}$ by

$$\{e^1\wedge e^2, e^1\wedge e^3, e^1\wedge e^4, e^3\wedge e^4, e^4\wedge e^2, e^2\wedge e^3\} \tag{2}$$

with the following nonzero inner products

$$\begin{aligned}(e^1\wedge e^2, e^1\wedge e^2) &= -(e^1\wedge e^3, e^1\wedge e^3)\\ &= -(e^1\wedge e^4, e^1\wedge e^4) = (e^3\wedge e^4, e^3\wedge e^4) = -(e^4\wedge e^2, e^4\wedge e^2)\\ &= -(e^2\wedge e^3, e^2\wedge e^3) = +1.\end{aligned} \tag{3}$$

Thus, Λ^2 is a six-dimensional vector space with the inner product of signature $(+ - - + - -)$.

The pseudo-orthogonal group O(2,2) acts on Λ^p isometrically with respect to the inner product. Hereafter we consider only SO(2,2). There is a local isomorphism $\mathrm{SO}(2,2)_{\text{local}} = \mathrm{SO}(1,2)\times\mathrm{SO}(1,2)$, which corresponds to the Lie algebra decomposition

$$\mathrm{so}(2,2) = \mathrm{so}(1,2) + \mathrm{so}(1,2). \tag{4}$$

This implies that Λ^2 can be split into the direct sum of two three-dimensional vector spaces of signature $(+ - -)$. This decomposition is given explicitly by using the Hodge star operation defined below.

The Hodge star operation, denoted by $*$, is a linear transformation from Λ^p onto Λ^{4-p} such that

$$a\wedge *b = (a,b)w, \quad a, b\in\Lambda^p, \tag{5}$$

where w is the volume form determined by the inner product and the orientation of the manifold. Thus, for $p = 2$, the star operation transforms Λ^2 onto itself, and decomposes it into three-dimensional eigenspaces Λ^2_+, Λ^2_- of $*$ with eigenvalues $+1$, -1, respectively:

$$\Lambda^2 = \Lambda^2_+ + \Lambda^2_-, \tag{6}$$

where both subspaces are endowed with an inner product invariant under actions of SO(1,2). This suggests that it is convenient to introduce a suitable basis in the subspaces. Denote such an orthonormal basis of Λ^2_+, Λ^2_- by $\{E^1_+, E^2_+, E^3_+\}$, $\{E^1_-, E^2_-, E^3_-\}$, respectively. They have the following properties for the star operator,

$$*E^i_+ = E^i_+, \quad *E^i_- = -E^i_-, \quad i = 1,2,3, \tag{7}$$

and the nonzero wedge and inner products

$$E^i_+ \wedge E^i_+ = -E^i_- \wedge E^i_- = \hat{\epsilon}^i w, \quad (E^i_\pm, E^i_\pm) = \hat{\epsilon}^i, \tag{8}$$

where $\hat{\epsilon}^1 = -\hat{\epsilon}^2 = -\hat{\epsilon}^3 = +1$.

The curvature R is expressed by a real 6×6 matrix as a linear transformation in Λ^2. Relative to $\{E^i_+, E^i_-\}$, R is decomposed into four disjoint parts:

$$R = R_+ + R_- + R_{+-} + R_{-+}, \tag{9}$$

where $R_\pm \in \mathrm{End}(\Lambda^2_\pm)$, $R_{+-} \in \mathrm{Hom}(\Lambda^2_+, \Lambda^2_-)$, $R_{-+} \in \mathrm{Hom}(\Lambda^2_-, \Lambda^2_+)$. A curvature 2-form $\Omega = \Omega^+ + \Omega^-$ relative to $\{E^i_+, E^i_-\}$ is defined by

$$\Omega^{\pm i} = \sum_{j=1}^{3} (R^{\pm i, +j} E^j_+ + R^{\pm i, -j} E^j_-), \tag{10}$$

where the $\Omega^{\pm i}$'s are the components of vectors $\Omega^\pm = (\Omega^{\pm 1}, \Omega^{\pm 2}, \Omega^{\pm 3})$ and the $R^{\pm i, \pm j}$'s are the components of R.

Thus for a 4-manifold of signature $(+ + - -)$, there are two ad(SO(2,2))-invariant 4-forms $*\Omega\wedge\Omega$, $\Omega\wedge\Omega$, which are reduced to ad(SO(1,2))-invariant 4-forms $\mathbf{\Omega}_+$, $\mathbf{\Omega}_-$ as follows.

$$*\Omega\wedge\Omega = \mathbf{\Omega}_+ - \mathbf{\Omega}_-, \quad \Omega\wedge\Omega = \mathbf{\Omega}_+ + \mathbf{\Omega}_- \tag{11}$$

where

$$\mathbf{\Omega}_+ = \Omega^+\wedge\Omega^+ = \sum_{i=1}^{3} \hat{\epsilon}^i \Omega^{+i}\wedge\Omega^{+i}, \tag{12a}$$

$$\mathbf{\Omega}_- = \Omega^-\wedge\Omega^- = \sum_{i=1}^{3} \hat{\epsilon}^i \Omega^{-i}\wedge\Omega^{-i}. \tag{12b}$$

Hereafter, we focus our attention to the normal forms of the curvature of an Einstein 4-manifold of signature $(+ + - -)$. Let S be a constant scalar curvature of the Einstein manifold. It should be noted that the curvature R relative to $\{E^i_+, E^i_-\}$ is of Einstein iff $R_{+-} = R_{-+} = 0$.[4,10] Thus the curvature of an Einstein manifold, $R = R_+ + R_-$, takes the form

$$R_+ = \begin{bmatrix} P_+ & 0 \\ 0 & 0 \end{bmatrix}, \quad R_- = \begin{bmatrix} 0 & 0 \\ 0 & P_- \end{bmatrix}, \tag{13}$$

where $P_\sigma = (R^{\sigma i, \sigma j})$, $\sigma = +, -$, are 3×3 matrices of the form

$$P_\sigma = \begin{bmatrix} a_1 + \sigma\alpha_1 & b - \sigma\beta & c - \sigma\gamma \\ -b - \sigma\beta & -a_2 + \sigma\alpha_2 & d + \sigma\delta \\ -c - \sigma\gamma & d + \sigma\delta & -a_3 + \sigma\alpha_3 \end{bmatrix} \tag{14}$$

with constraints

$$\tfrac{1}{2}\mathrm{Tr}R = \mathrm{Tr}P_+ = \mathrm{Tr}P_- = \sum_{i=1}^{3} \hat{\epsilon}^i a_i = \frac{S}{4}, \tag{15a}$$

$$\sum_{i=1}^{3} \alpha_i = 0. \tag{15b}$$

Analogous to the works of Petrov[8,9] and Singer and Thorpe,[10] we obtain normal forms of the curvature.

Proposition 1: For an Einstein 4-manifold of signature $(+ + - -)$, the curvature tensor takes one of the following three forms:

$$\text{(i)}P_\sigma = \begin{bmatrix} \mu_1 + \sigma\nu_1 & 0 & 0 \\ 0 & -\mu_2 + \sigma\nu_2 & 0 \\ 0 & -0 & \mu_3 + \sigma\nu_3 \end{bmatrix} \tag{16a}$$

with $\Sigma^3_{i=1} \hat{\epsilon}^i \mu_i = S/4$, $\Sigma^3_{i=1} \nu_i = 0$.

$$\text{(ii)}P_\sigma = \begin{bmatrix} \mu_2 + \sigma(\frac{1}{2}\nu_1 + \nu_2) & -\frac{1}{2}\sigma\nu_1 & 0 \\ -\frac{1}{2}\sigma\nu_1 & -\mu_2 + \sigma(\frac{1}{2}\nu_1 - \nu_2) & 0 \\ 0 & 0 & \frac{1}{4}S - \sigma\nu_1 \end{bmatrix},$$

$$\nu_1 \neq 0. \tag{16b}$$

$$\text{(iii)}P_\sigma = \begin{bmatrix} -\frac{1}{4}S & -\sigma\beta & 0 \\ -\sigma\beta & \frac{1}{4}S & \sigma\beta \\ 0 & \sigma\beta & \frac{1}{4}S \end{bmatrix}, \quad \beta \neq 0. \tag{16c}$$

Proof: Consider a latent equation

$$(R - \lambda g)W = 0, \quad W \in \Lambda^2, \tag{17}$$

where $g = \mathrm{diag}[+1, -1, -1, +1, -1, -1]$. This equation is equivalent to two latent equations of 3×3 matrices

$$(P_\sigma - \lambda g_0)W_\sigma = 0, \quad W_\sigma \in \Lambda^2_\sigma, \tag{18}$$

where $g_0 = \mathrm{diag}[+1, -1, -1]$. Due to Petrov,[9] the symbol σ of elements of P_σ must satisfy $\sigma^2 = 1$, and the number $z = a + \sigma b$ is called a duplex number with its conjugate $\bar{z} = a - \sigma b$. Thus eigenvalues are obtained in the forms of duplex number from the equation

$$|P_\sigma - \lambda g_0| = 0. \tag{19}$$

Depending on the number of independent eigenvectors, we have three different cases for the equation. For each type, we must consider the following equations for the eigenvalues λ_i's and eigenvectors W_i's of Λ^2_+:

$$\text{(i)}P_+ W_i = \lambda_i W_i \quad (i = 1,2,3), \tag{20a}$$

where W_i can be taken as E^i_+.

$$\text{(ii)}P_+ W_i = \lambda_i W_i \quad (i = 1,2), \quad P_+ W_3 = \lambda_2 W_3 + \kappa W_2 \quad (\kappa \neq 0), \tag{20b}$$

where the W_i's can be taken as $W_1 = E^1_+$, $W_2 = E^1_+ + E^2_+$, $W_3 = E^1_+ - E^2_+$.

$$\text{(iii)}P_+ W_1 = \lambda_1 W_1, \quad P_+ W_2 = \lambda_1 W_2 + \rho W_1 \quad (\rho \neq 0),$$
$$P_+ W_3 = \lambda_1 W_3 + \tau W_2 \quad (\tau \neq 0), \tag{20c}$$

where the W_i's can be taken as $W_1 = E^1_+ + E^3_+$, $W_2 = E^2_+$, $W_3 = E^1_+ - E^3_+$. Since the P_- is obtained from P_+ by the duplex conjugation, these equations yield the three types of explicit forms of P_σ.□

The Einstein 4-manifold of signature $(+ + - -)$ is quite similar to that of a Lorentz metric in that there are three types of normal forms of the curvature. On the other hand, there is another similarity between a 4-manifold of signature $(+ + - -)$ and that of a Riemannian metric, since the Lie algebras so(2,2) and so(4) have similar isomorphisms:

$$\mathrm{so}(2,2)=\mathrm{so}(1,2)+\mathrm{so}(1,2), \tag{4}$$

$$\mathrm{so}(4)=\mathrm{so}(3)+\mathrm{so}(3), \tag{21}$$

respectively.

III. EULER CHARACTERISTICS

For a compact oriented pseudo-Riemannian manifold of any dimension and signature, Chern[7] obtained the generalized version of the Gauss–Bonnet formula. The arguments developed here are based upon this work. For a manifold of signature

$$(\underbrace{+1,\ldots,+1}_{p},\quad \underbrace{-1,\ldots,-1}_{q}),$$

the Euler characteristic vanishes if at least one of p,q is odd. Thus for the compact 4-manifold of $p=q=2$, the Euler characteristic may be nontrivial and is given by integrating the following form over the manifold:

$$(1/8\pi^2)^*\Omega\wedge\Omega=(1/8\pi^2)(\mathbf{\Omega}_+-\mathbf{\Omega}_-). \tag{22}$$

The analog of the first Pontrjagin class, referred to as the pseudo-Pontrjagin class, is given by integrating the following form over the manifold:

$$(1/4\pi^2)\Omega\wedge\Omega=(1/4\pi^2)(\mathbf{\Omega}_++\mathbf{\Omega}_-). \tag{23}$$

For the compact oriented Einstein 4-manifold of signature $(++--)$, denoted by M, we have the 4-forms $\mathbf{\Omega}_+$, $\mathbf{\Omega}_-$ by using the normal forms of Proposition 1 as follows:

$$\text{for } M_1{:}\ \mathbf{\Omega}_\pm=\pm\left[\sum_{i=1}^{3}(\mu_i\pm\nu_i)^2\right]w, \tag{24a}$$

with constraints

$$\sum_{i=1}^{3}\hat{\epsilon}^i\mu_i=\frac{S}{4},\quad \sum_{i=1}^{3}\nu_i=0, \tag{*}$$

$$\text{for } M_2{:}\quad \mathbf{\Omega}_\pm=\pm\left[(S/4\mp\nu_1)^2+2(\mu_2\pm\nu_2)^2\right]w_1,\quad \nu_1\neq 0, \tag{24b}$$

$$\text{for } M_3{:}\quad \mathbf{\Omega}_+=-\mathbf{\Omega}_-=\tfrac{3}{16}S^2, \tag{24c}$$

where M_i is the manifold M whose curvature is of type i

Using these expressions, we obtain explicit forms of the Euler characteristic χ and the pseudo-Pontrjagin class, denoted by $\bar{p}_1$.

Proposition 2: For M, the Euler characteristic $\chi[M]$ and the pseudo-Pontrjagin class $\bar{p}_1[M]$ are given as follows:

$$\chi[M_1]=\frac{1}{4\pi^2}\int_{M_1}\sum_{i=1}^{3}(\mu_i^2+\nu_i^2)w,\quad \text{with}(*),$$

$$=\frac{S^2}{2^6\pi^2}\mathrm{vol}(M_1)+\frac{S}{2^3\pi^2}I+\frac{1}{2^2\pi^2}J, \tag{25a}$$

where μ_1, ν_1 are eliminated by the constraints (*) and

$$I=\int_{M_1}(\mu_2+\mu_3)w,\quad J=\int_{M_1}\sum_{i,j=2,3}(\mu_i\mu_j+\nu_i\nu_j)w,$$

$$\chi[M_2]=\frac{S^2}{2^6\pi^2}\mathrm{vol}(M_2)+\frac{1}{2^2\pi^2}\int_{M_2}(2\mu_2^2+\nu_1^2+2\nu_2^2)w,\quad \nu_1\neq 0, \tag{25b}$$

$$\chi[M_3]=\frac{3S^2}{2^6\pi^2}\mathrm{vol}(M_3). \tag{25c}$$

$$\bar{p}_1[M_1]=\frac{1}{\pi^2}\int_{M_1}\Big(\sum_{i=1}^{3}\mu_i\nu_i\Big)w,\quad \text{with}(*),$$

$$=\frac{S}{4\pi^2}\int_{M_1}\nu_1 w-\frac{1}{\pi^2}\int_{M_1}(\mu_3\nu_2+\mu_2\nu_3)w, \tag{26a}$$

$$\bar{p}_1[M_2]=-\frac{S}{4\pi^2}\int_{M_2}\nu_1 w+\frac{1}{2\pi^2}\int_{M_2}(\mu_2\nu_2)w,\quad \nu_1\neq 0, \tag{26b}$$

$$\bar{p}_1[M_3]=0. \tag{26c}$$

Proof: These results are obtained by straightforward calculation.□

Thus the Euler characteristics are quadratic forms of S. For the second type the Euler characteristic has no linear term of S, and for the third type it has only a quadratic term of S. The pseudo-Pontrjagin classes, however, are the linear forms of S, except for $\bar{p}_1[M_3]$, which is identically zero. The next proposition gives an inequality between $\chi[M]$ and $\bar{p}_1[M]$. This inequality directly follows from the above explicit forms and is an analog of Hitchin's inequality.[2]

Proposition 3: For M we have

$$\chi[M]\geqslant\tfrac{1}{2}|\bar{p}_1[M]|. \tag{27}$$

The equality occurs if $\mu_i=\pm\nu_i$ for all $i=1,2,3$ for M_1, if $\nu_1=\pm S/4\,(\neq 0)$, $\mu_2=\pm\nu_2$ for M_2, and iff $S=0$ for M_3.

Proof: This is elementary. It is to be noted that for M_3 both sides of the inequality vanish when the equality occurs.□

In order to prove the main theorem, it is necessary to use the following two lemmas.

Lemma A[6]: A compact manifold admits an everywhere defined, continuous, nonsingular, quadratic form of signature k if and only if it admits a continuous field of tangent k-planes.

Lemma B[11]: For a compact oriented $4n$-manifold admitting a tangent field of 2-planes, the Euler characteristic of the manifold is even and is congruent to the index modulo 4.

Now let us state the main theorem.

Theorem 4: For a compact oriented Einstein 4-manifold M of signature $(++--)$, the Euler characteristic $\chi[M]$ is nonnegative and even and is congruent to the index of M modulo 4. To be more concrete, $\chi[M_1]$ vanishes iff M_1 is flat; $\chi[M_2]$ is strictly positive; and $\chi[M_3]$ vanishes iff M_3 is Ricci flat.

Proof: For the property that $\chi[M]\geqslant 0$, it is clear from the explicit forms. For M_1, $\chi[M_1]=0$ iff $\mu_i=\nu_i=0$ for all i. This condition implies that the manifold is flat. For both M_2 and M_3, the manifolds are never flat. Since for M_2 there is a nonzero factor ν_1, we have $\chi[M_2]>0$. For M_3, it is clear that $\chi[M_3]=0$ iff $S=0$. For the other properties that $\chi[M]$ is even and congruent to the index modulo 4, it is a direct consequence of Lemmas A and B. This completes the proof. □

This theorem has the following corollary.

Corollary 5: (i) $\chi[M_2]\geqslant 2$,

(ii) $\chi[M_2]\geqslant 2$ if M_i is not flat,

(iii) $\chi[M_3]\geqslant 2$ if $S\neq 0$.

The next proposition is concerned with the volume of M_3.

Proposition 6: If $S\neq 0$, then there is a lower bound for the volume of M_3,

$$\mathrm{vol}(M_3) \geqslant 2^7\pi^2/3S^2 \tag{28}$$

with equality iff $\chi[M_3] = 2$.

Proof: This is derived from (iii) of Corollary 5. □

For M_1, M_2, however, no such lower bound exists. The following proposition is also concerned with the volume.

Proposition 7: Consider three manifolds M_i of type i ($i = 1,2,3$) whose scalar curvatures are equal and nonzero and whose Euler characteristics coincide with each other. Then the volumes of the manifolds satisfy the inequalities

$$\text{(i) } \mathrm{vol}(M_2) < 3\mathrm{vol}(M_3), \tag{29a}$$

$$\text{(ii) } \mathrm{vol}(M_1) \leqslant 3\mathrm{vol}(M_3) \text{ if } S\cdot I \geqslant 0, \tag{29b}$$

where the equality occurs iff $I = J = 0$.

Proof: By equating $\chi[M_1]$, $\chi[M_2]$, and $\chi[M_3]$ in Proposition 3, we have two relations

(i) $3\mathrm{vol}(M_3) = \mathrm{vol}(M_2) + 2^4S^{-2}K$,

(ii) $3\mathrm{vol}(M_3) = \mathrm{vol}(M_1) + 2^3S^{-1}I + 2^4S^{-2}J$,

where

$$K = \int_{M_2}(2\mu_2^2 + \nu_1^2 + 2\nu_2^2)w > 0, \quad J \geqslant 0. \tag{30}$$

These are led to the desired inequalities.□

For the Betti numbers, we have

Proposition 8: For the manifold M stated in Theorem 4, the second Betti number is even. If $S \neq 0$ and the second Betti number is zero, then the first number is zero.

Proof: Let b_k denote the k-th Betti number of M. The Euler characteristic is expressed by the duality $b_n = b_{4-n}$ as

$$\chi[M] = 2b_0 - 2b_1 + b_2. \tag{31}$$

The first part of the proposition is trivial, since $\chi[M]$ is even. Since M is connected, we have $b_0 = 1$. Then setting $b_2 = 0$, we have $\chi[M] = 2 - 2b_1 \leqslant 2$, and accordingly $\chi[M] \geqslant 2$ from Corollary 5. Thus we obtain $b_1 = 0$.□

Remarks: (i) Even for the Reimannian case of compact Einstein 4-manifolds, there are few known examples. Hitchin[2] showed that a $K3$ surface admits an Einstein metric and that the manifold $X_n = nCP^2$ ($n \geqslant 4$) is a simply connected manifold which does not carry an Einstein metric. By Theorem 4, an X_n does not carry a $(+ + - -)$ metric since $\chi[X_n] = n + 2$ and the index $\tau[X_n] = n$ for $n \geqslant 1$. Such a metric is also forbidden on a 4-sphere S^4.

(ii) Simple example: For $X = S^2 \times S^2$, we have $\chi[X] = 4$ and $\tau[X] = 0$. The mainfold X admits an Einstein metric of signature $(+ + - -)$,

$$ds^2 = a^2(d\xi + \sin^2\xi\, d\phi^2 - d\eta^2 - \sin^2\eta\, d\psi^2), \tag{32}$$

where $0 \leqslant \xi, \eta \leqslant \pi$, $0 \leqslant \phi, \psi \leqslant 2\pi$, and $a \neq 0$. For X, we have $\bar{p}_1[X] = 0$, which coincides with $\tau[X] = 0$. The metric is of type 1.

(iii) It is an open question whether or not the pseudo-Pontrjagin class $\bar{p}_1$ defined on the pseudo-Riemannian bundle over a manifold coincides with the first Pontrjagin class p_1 defined on the tangent bundle over the manifold. In other words, it is not known whether the Hirzebruch relation $\tau[M] = \frac{1}{3}p_1[M]$ can be generalized for the pseudo-Pontrjagin class $\bar{p}_1$. This problem may be contrasted to the generalized Gauss–Bonnet formula of Chern.

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On the substructure of the classical observables x^α, p_α, and $J^{\alpha\beta}$

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The position, momentum, and angular momentum (spin + orbital) of a classical massive magnetic dipole particle are constructed from certain pairs of $\overline{O(3,3)}$ spinors and a scalar σ. These spinor pairs (and also σ) are endowed with a translation transformation law (which is fundamentally different from that of twistors), and are given the name hyperspinors. An action of the covering group of the Poincaré group is defined on hyperspinors and σ. Equations of motion for these hyperspinors and σ are proposed, special cases of which lead to the Lorentz force law for the momentum and the BMT (Bargmann, Michel, and Telegdi) equation for the Pauli–Lubanski pseudovector. A generalization to include SU(N) internal degrees of freedom in this model is suggested.

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INTRODUCTION

Can one ascribe a substructure to Minkowski space-time M_4? At present no one knows, and much effort is focused on this problem, for the resolution of this question may lead to the elimination of the divergences that appear in most local quantum field theories, and perhaps even to the unification of gravity with the other nonabelian gauge theories. However, progress has been made toward an answer to this question, and to mention one important example, Qadir[1] has shown that the coordinates $x^\alpha(p)$ of a point $p\in M_4$ may be explicitly constructed from a pair of twistors that are members of a twistor quadrad.

A related question, founded in operational and not purely nominal concepts, is whether or not one can attribute an underlying substructure to the position in M_4 of a massive point particle. The answer to this question is that this can be done, at least when one neglects gravity. It has been shown[2] that the position in M_4 of a free classical massive point particle may be endowed with an intrinsic substructure; the classical observable "position" may be constructed from certain twistors that describe not only the position, but also the momentum and angular momentum (spin + orbital) of the particle. [Of course, when one excludes interactions the concepts "point in space-time" and "position of point particle in space-time" coincide, but it seems that the formalism in Ref. 2 can also be utilized when one is modeling the dynamical evolution of massive particles under the influence of nongravitational interactions; in particular, the only Lorentz covariant, constraint-preserving (see below) equations of motion for these twistors are not the trivial no-interaction equations.]

In this paper it is shown how the position in M_4 of an interacting massive point particle may be constructed from a geometrical object that we call a hyperspinor. The hyperspinor formalism has several advantages over the twistor formalism of Ref. 2. There the principal bundle of orthogonal frames over M_4 is constructed from certain pairs of real-valued eight-component $\overline{O(3,3)}$ [the universal covering group of O(3,3)] spinors. These $\overline{O(3,3)}$ spinors are endowed with the homogeneous twistor translation law, and are referred to generically as twistors. This construction is rather unwieldy, because an arbitrary pair of real $\overline{O(3,3)}$ spinors has sixteen independent components, whereas the orthogonal frame bundle over M_4 is eleven-dimensional; therefore five independent constraints must be imposed on a pair of $\overline{O(3,3)}$ spinors in order to formulate the one-to-one correspondence between the orthogonal frame bundle over M_4 and (certain) pairs of $\overline{O(3,3)}$ spinors. These constraints complicate the formulation of classical and quantum dynamical schemes for the time evolution of these twisters. However, if one gives up the twistorlike translation law for these $\overline{O(3,3)}$ spinors, and instead endows these spinors with a (slightly) more complicated translation transformation law, then most of the above-mentioned constraints never arise. A pair of $\overline{O(3,3)}$ spinors satisfying certain conditions and transforming under translation according to the new translation transformation law alluded to above is a hyperspinor. In the following we shall construct the coordinates $x^\alpha(p)$, $p\in M_4$, momentum, and angular momentum of a massive particle possessing an intrinsic magnetic dipole moment from hyperspinors and a scalar σ, and also define classical equations of motion for these hyperspinors and σ which yield the usual Lorentz force law and BMT (Bargmann, Michel, and Telegdi) equations for the Pauli–Lubanski pseudovector. In addition, we indicate how one might incorporate SU(N) internal degrees of freedom into this formalism.

CONSTRUCTION OF CLASSICAL OBSERVABLES[3,4]

In order to make this paper more or less self contained, we begin this section by quoting the definitions and conventions of Ref. 2 that are relevant to our later work.

Let ψ denote a real column matrix with eight rows (row indices are suppressed) which coordinizes a real eight-dimensional vector space S_8. $\overline{O(3,3)}$ acts on S_8 on the left as a group of automorphisms that preserves a certain bilinear form; ψ transforms as a spinor under a real 8×8 irreducible

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representation of $\overline{O(3,3)}$. Write

$$\psi = \begin{pmatrix} \lambda \\ \xi \end{pmatrix}, \tag{1}$$

where λ and ξ are real four-component $\overline{SO(3,3)}$ spinors. $\tilde{\xi}$ ($\sim$ denotes transpose) transforms inversely to λ under $\overline{SO(3,3)}$.

Let γ^α ($\alpha,\beta,\cdots = 1,2,3,4$) be a real 4×4 irreducible (Majorana) representation of the Dirac matrices, where

$$\gamma^\alpha\gamma^\beta + \gamma^\beta\gamma^\alpha = 2\gamma_0 g^{\alpha\beta}, \tag{2}$$

$$g_{\alpha\beta} = g^{\alpha\beta} = \text{diag}(1,1,1,-1), \tag{3}$$

and γ_0 is the 4×4 unit matrix. Define

$$\gamma^5 = -(1/4!)\epsilon_{\alpha\beta\mu\nu}\gamma^\alpha\gamma^\beta\gamma^\mu\gamma^\nu = -\gamma^1\gamma^2\gamma^3\gamma^4, \tag{4}$$

$$\epsilon = \gamma^4\gamma^5, \tag{5}$$

(note that ϵ,γ^4, and γ^5 are skew-symmetric and have square equal to $-\gamma_0$) and

$$S^{\alpha\beta} = -\tfrac{1}{4}(\gamma^\alpha\gamma^\beta - \gamma^\beta\gamma^\alpha) = -\tfrac{1}{4}[\gamma^\alpha,\gamma^\beta]. \tag{6}$$

Then

$$\gamma^5 S^{\alpha\beta} = \tfrac{1}{2}g^{\alpha\mu}g^{\beta\nu}\epsilon_{\mu\nu\lambda\sigma}S^{\lambda\sigma} \tag{7}$$

(there is a minus sign error in Eq. (99) of Ref. 3),

$$\tilde{\gamma}^\alpha\gamma^4 = -\gamma^4\gamma^\alpha, \tag{8}$$

$$\tilde{\gamma}^\alpha\epsilon = \epsilon\gamma^\alpha, \tag{9}$$

$$\tilde{S}^{\alpha\beta}\gamma^4 = -\gamma^4 S^{\alpha\beta}, \tag{10}$$

$$\tilde{S}^{\alpha\beta}\epsilon = -\epsilon S^{\alpha\beta}, \tag{11}$$

$$[S^{\alpha\beta},\gamma_\mu] = \delta^\alpha_\mu\gamma^\beta - \delta^\beta_\mu\gamma^\alpha \tag{12}$$

and

$$[S^{\alpha\beta},S^{\mu\nu}] = g^{\alpha\mu}S^{\beta\nu} - g^{\alpha\nu}S^{\beta\mu} - g^{\beta\mu}S^{\alpha\nu} + g^{\beta\nu}S^{\alpha\mu}. \tag{13}$$

The γ matrices satisfy[2,3]

$$-\gamma^4\gamma^\alpha\lambda\tilde{\xi}\gamma_\alpha\gamma^4 = \gamma_0\tilde{\xi}\lambda + \xi\tilde{\lambda} - \gamma^5\tilde{\xi}\gamma^5\lambda + \gamma^5\xi\tilde{\lambda}\gamma^5, \tag{14}$$

$$-\gamma^\alpha\gamma^4\xi\tilde{\lambda}\gamma^4\gamma_\alpha = \gamma_0\tilde{\xi}\lambda + \lambda\tilde{\xi} + \gamma^5\tilde{\xi}\gamma^5\lambda + \gamma^5\lambda\tilde{\xi}\gamma^5; \tag{15}$$

in particular

$$-\gamma_\alpha\gamma^4\xi\tilde{\xi}\gamma^\alpha = \gamma^4\xi\tilde{\xi} - \epsilon\xi\tilde{\xi}\gamma^5 \tag{16}$$

and

$$-\gamma_\alpha\lambda\tilde{\lambda}\gamma^4\gamma^\alpha = \lambda\tilde{\lambda}\gamma^4 + \gamma^5\lambda\tilde{\lambda}\epsilon. \tag{17}$$

Let Γ^A ($A,B,\cdots = 1,\ldots,6$) be six real matrices which generate an irreducible representation of the Clifford algebra C_6:

$$\Gamma^A\Gamma^B + \Gamma^B\Gamma^A = 2g^{AB}, \tag{18}$$

where

$$g_{AB} = g^{AB} = \text{diag}(1,1,1,-1,-1,-1) \tag{19}$$

[The 8×8 unit matrix is suppressed on the right-hand side of Eq. (18)]. Define

$$\Gamma^7 = (1/6!)\epsilon_{ABCDEF}\Gamma^A\Gamma^B\Gamma^C\Gamma^D\Gamma^E\Gamma^F; \tag{20}$$

then

$$\Gamma^A\Gamma^7 + \Gamma^7\Gamma^A = 0 \tag{21}$$

and

$$(\Gamma^7)^2 = 1. \tag{22}$$

A particular representation of the Γ matrices is

$$\Gamma^\alpha = \begin{pmatrix} 0 & \gamma^\alpha\epsilon \\ -\epsilon\gamma^\alpha & 0 \end{pmatrix}, \tag{23}$$

$$\Gamma^5 = \begin{pmatrix} 0 & \gamma^5\epsilon \\ -\epsilon\gamma^5 & 0 \end{pmatrix}, \tag{24}$$

$$\Gamma^6 = \begin{pmatrix} 0 & -\epsilon \\ -\epsilon & 0 \end{pmatrix}, \tag{25}$$

and

$$\Gamma^7 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{26}$$

The generators of $\overline{SO(3,3)}$ are

$$M^{AB} = -\tfrac{1}{4}[\Gamma^A,\Gamma^B], \tag{27}$$

and they satisfy

$$[M^{AB},\Gamma_R] = \delta^A_R\Gamma^B - \delta^B_R\Gamma^A \tag{28}$$

and

$$[M^{AB},M^{RS}] = g^{AR}M^{BS} - g^{AS}M^{BR} - g^{BR}M^{AS} + g^{BS}M^{AR}. \tag{29}$$

In the representation of Eqs. (23–26) the $M^{\alpha\beta}$ are given by

$$M^{\alpha\beta} = \begin{pmatrix} S^{\alpha\beta} & 0 \\ 0 & -\tilde{S}^{\alpha\beta} \end{pmatrix}, \tag{30}$$

and an element M of $\overline{SO(3,1)}$ (such that $\psi \rightarrow \psi' = M\psi$) is given by

$$M = \begin{pmatrix} S & 0 \\ 0 & \tilde{S}^{-1} \end{pmatrix}, \tag{31}$$

where

$$S = \exp\{\tfrac{1}{2}\omega_{\alpha\beta}S^{\alpha\beta}\} \tag{32}$$

and the $\omega_{\alpha\beta} = -\omega_{\beta\alpha}$ are six real parameters. (The transformation properties of ψ under $\overline{O(3,1)}$ are discussed in Ref. 3.)

The skew-symmetric metric spinor of rank two, Ω, may be defined by

$$\tilde{\Gamma}^A\Omega = \Omega\Gamma^A; \tag{33}$$

then

$$\tilde{\Gamma}^7\Omega = -\Omega\Gamma^7 \tag{34}$$

and

$$\tilde{M}^{AB}\Omega = -\Omega M^{AB}. \tag{35}$$

In the above representation Ω may be chosen to be

$$\Omega = \Gamma^1\Gamma^2\Gamma^3 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{36}$$

Let us now restrict our attention to the seven-dimensional submanifold of S_8 defined by

$$\tilde{\xi}\lambda = 0 \tag{37}$$

and

$$\tilde{\xi}\gamma^5\lambda \neq 0 \tag{38}$$

In Ref. 3 it is shown that $\overline{O(3,3)}$ spinors lying in this subset of S_8 describe massive magnetic dipole particles, such as electrons. There it is also shown that a $\overline{O(3,3)}$ spinor ψ satisfying Eqs. (37) and (38) determines two linearly independent future-pointing null vectors n^α and l^α, a spin tensor $\Sigma^{\alpha\beta}$, an orthogonal tetrad $e^\alpha_{(\mu)}$, and a scalar N. These are defined in terms of ψ according to

$$e^\alpha_{(1)} = -\tfrac{1}{2}\tilde{\xi}\gamma^\alpha\gamma^5\lambda = -\tfrac{1}{2}\tilde{\psi}\Omega M^{\alpha 5}\psi, \quad (39)$$

$$e^\alpha_{(2)} = -\tfrac{1}{2}\tilde{\xi}\gamma^\alpha\lambda = -\tfrac{1}{2}\tilde{\psi}\Omega M^{\alpha 6}\psi, \quad (40)$$

$$\Sigma^{\alpha\beta} = \tilde{\xi}S^{\alpha\beta}\lambda = -\tfrac{1}{2}\tilde{\psi}\Omega M^{\alpha\beta}\psi, \quad (41)$$

$$N = -\tfrac{1}{2}\tilde{\xi}\gamma^5\lambda = -\tfrac{1}{2}\tilde{\psi}\Omega M^{56}\psi, \quad (42)$$

$$n^\alpha = -\tilde{\lambda}\gamma^4\gamma^\alpha\lambda, \quad (43)$$

$$l^\alpha = -\tilde{\xi}\gamma^\alpha\gamma^4\xi, \quad (44)$$

$$e^\alpha_{(3)} = \tfrac{1}{4}(n^\alpha - l^\alpha) = -\tfrac{1}{4}\tilde{\psi}\Gamma^4\Gamma^\alpha\Gamma^7\psi, \quad (45)$$

and

$$e^\alpha_{(4)} = \tfrac{1}{4}(n^\alpha + l^\alpha) = -\tfrac{1}{4}\tilde{\psi}\Gamma^4\Gamma^\alpha\psi. \quad (46)$$

The $e^\alpha_{(\mu)}$ satisfy[3]

$$e^\alpha_{(\mu)}e_{(\nu)\alpha} = N^2\eta_{(\mu)(\nu)}, \quad (47)$$

where

$$\eta_{(\mu)(\nu)} = \text{diag}(1,1,1,-1). \quad (48)$$

In particular, the unit (timelike) four-velocity v^α, defined by

$$v^\alpha = N^{-1}e^\alpha_{(4)} \quad (49)$$

satisfies

$$v^\alpha v_\alpha = -1. \quad (50)$$

Put

$$v = \gamma_\alpha v^\alpha. \quad (51)$$

Then using Eqs. (14)–(17) one can easily show that

$$\xi = \epsilon v\lambda \quad (52)$$

and

$$\lambda = v\epsilon\xi \quad (53)$$

are identities when ψ satisfies Eqs. (37) and (38).

Henceforth we shall assume that ψ satisfies Eqs. (37) and (38). Let $\psi_1 = \begin{pmatrix}\lambda_1\\ \xi_1\end{pmatrix} \in S_8$. We shall arrange that (ψ,ψ_1) has only $(8-1)+4 = 11$ independent components by defining ξ_1 in terms of λ_1 and ψ according to

$$\xi_1 = \epsilon v\lambda_1, \quad (54)$$

where v is defined in terms of ψ in Eq. (51). Upon multiplying Eq. (54) by $v\epsilon$ one finds that, analogous to Eq. (53),

$$\lambda_1 = v\epsilon\xi_1. \quad (55)$$

A result from Ref. 3 is that if ψ_1 satisfies Eqs. (54) and (55), then $-\frac{1}{4}\tilde{\psi}_1\Gamma^4\Gamma^\alpha\psi_1$ [cf. Eq. (46)] is parallel to v^α.

Note that for nonzero λ_1,

$$\tilde{\xi}_1\lambda_1 = -\tilde{\lambda}_1\epsilon v\lambda_1 = 0 \quad (56)$$

(because $\widetilde{\epsilon v} = -\epsilon v$) and

$$\tilde{\xi}_1\gamma^5\lambda_1 = -\tilde{\lambda}_1\gamma^4\gamma_\alpha\lambda_1 v^\alpha \neq 0 \quad (57)$$

(because $-\tilde{\lambda}_1\gamma^4\gamma^\alpha\lambda_1$ is a null vector and v^α is timelike).

Under $\overline{SO(3,3)}$,

$$\lambda \to \lambda' = S\lambda; \quad \lambda_1 \to \lambda_1' = S\lambda_1, \quad (58)$$

and

$$\xi \to \xi' = \tilde{S}^{-1}\xi; \quad \xi_1 \to \xi_1' = \tilde{S}^{-1}\xi_1, \quad (59)$$

where S is given by Eq. (32). Further,

$$v^\alpha \to v'^\alpha = \Lambda^\alpha{}_\beta v^\beta, \quad (60)$$

where

$$\Lambda^\alpha{}_\beta = \tfrac{1}{4}\,\text{tr}S^{-1}\gamma^\alpha S\gamma_\beta = (e^{-\omega})^\alpha{}_\beta, \quad (61)$$

since

$$\gamma^\alpha = \Lambda^\alpha{}_\beta S\gamma^\beta S^{-1} \quad (62)$$

under SO(3,1). Now $\xi_1' = \tilde{S}^{-1}\xi_1 = \tilde{S}^{-1}\epsilon v\lambda_1 = \epsilon S v\lambda_1$ [$\epsilon \to \epsilon' = \tilde{S}\epsilon S = \epsilon$ under $\overline{SO(3,1)}$, according to Eq. (11)] $= \epsilon S v S^{-1}\lambda_1' = \epsilon v'\lambda_1'$ (with $v' = \gamma_\alpha v'^\alpha$), so that the definition of Eq. (54) is independent of the Lorentz frame. We now define a left action on $S_8 \times S_8$ by T_4, the four-dimensional translation group, that also preserves the definition of Eq. (54).

Let b be a real 4×4 matrix that satisfies

$$\tilde{b}\epsilon = \epsilon b \quad (63)$$

and

$$\tilde{b}\gamma^4 = -\gamma^4 b\,. \quad (64)$$

Then b may be written uniquely as

$$b = b_\alpha\gamma^\alpha, \quad (65)$$

where the b^α are four real parameters given by

$$b^\alpha = \tfrac{1}{4}\,\text{tr}\gamma^\alpha b. \quad (66)$$

The translation action on $S_8 \times S_8$ is defined by

$$(\psi,\psi_1) \to (T_b\psi, T_b\psi_1) = (\psi, \psi_1 + b^\alpha T_\alpha\psi), \quad (67)$$

where

$$T^\alpha = v^\alpha\Gamma^7 + \Gamma^\alpha. \quad (68)$$

In four-component form,

$$\lambda \to T_b\lambda = \lambda, \quad (69)$$

$$\xi \to T_b\xi = \xi, \quad (70)$$

$$\lambda_1 \to T_b\lambda_1 = \lambda_1 + b\epsilon\xi + b\cdot v\lambda, \quad (71)$$

and

$$\xi_1 \to T_b\xi_1 = \xi_1 - \epsilon b\lambda - b\cdot v\xi, \quad (72)$$

where $b\cdot v = b_\alpha v^\alpha$. Note that this transformation law is nonlinear in ψ due to the terms $b\cdot v\lambda$ and $b\cdot v\xi$ which appear in Eqs. (71) and (72). A short calculation utilizing the identities of Eqs. (52) and (53) shows that Eqs. (54) and (55) are form-invariant under translation:

$$T_b\xi_1 = \epsilon v T_b\lambda_1 \quad (73)$$

and

$$T_b\lambda_1 = v\epsilon T_b\xi_1. \quad (74)$$

A pair of $\overline{O(3,3)}$ spinors (ψ,ψ_1) satisfying Eqs. (37), (38), (54), and (55) (and hence possessing eleven independent components), and furthermore endowed with the transformation law of Eq. (67) under translation will henceforth be said to constitute a *hyperspinor*.

The set of left actions on $S_8 \times S_8$ defined by Eq. (67) clearly commute with one another, and so provide a representation of T_4. In order to verify that we also have an action on $S_8 \times S_8$ by the semidirect product $\overline{\mathrm{SO}(3,3)} \circledS T_4$ (the universal covering group of the connected component of the Poincaré group), let us evaluate the commutator of $M^{\alpha\beta}$ and T_μ: for $M \in \overline{\mathrm{SO}(3,1)}$ and $T_b \in T_4$, $M(\psi,\psi_1) = (\psi',\psi_1') = (M\psi, M\psi_1); T_b M(\psi,\psi_1) = (T_b\psi', T_b\psi_1') = (\psi', \psi_1' + b^\mu T'_\mu \psi)$, where $T'_\mu = v'_\mu \Gamma^7 + \Gamma_\mu = \Lambda_{\mu\beta} v^\beta \Gamma^7 + \Gamma_\mu$; and $MT_b(\psi,\psi_1) = (M\psi, M\psi_1 + b^\mu M T_\mu M^{-1} M\psi) = (\psi', \psi_1' + b^\mu M T_\mu M^{-1}\psi')$. Therefore $(MT_b - T_b M)(\psi,\psi_1) = (0, b^\mu\{MT_\mu M^{-1} - T'_\mu\}\psi')$, and consequently

$$(MT_\mu - T_\mu M)(\psi,\psi_1) = (0, \{MT_\mu M^{-1} - T'_\mu\}\psi'). \quad (75)$$

Let M be an infinitesimal $\overline{\mathrm{SO}(3,1)}$ transformation, $M = 1 + \frac{1}{2}\omega_{\alpha\beta} M^{\alpha\beta} + \cdots$, where the $\omega_{\alpha\beta}$ now represent infinitesimal numbers; then $\Lambda^\alpha{}_\beta = \delta^\alpha{}_\beta - \omega^\alpha{}_\beta + \cdots$ and $T'_\mu = T_\mu - \omega_{\mu\beta} v^\beta \Gamma^7 + \cdots$. To first order in $\omega_{\alpha\beta}$, $(MT_\mu M^{-1} - T'_\mu)\psi'$ is $\frac{1}{2}\omega_{\alpha\beta}\{\delta^\alpha_\mu T^\beta - \delta^\beta_\mu T^\alpha\}\psi$, so that

$$[M^{\alpha\beta}, T_\mu](\psi,\psi_1) = (0, \quad \{\delta^\alpha_\mu T^\beta - \delta^\beta_\mu T^\alpha\}\psi). \quad (76)$$

Therefore the submanifold of $S_8 \times S_8$ in which the set of all hyperspinors lies is a carrier space for a (reducible) representation of the covering group of the (full) Poincaré group.

Equations (52) and (53) may be recast in a manifestly $\overline{\mathrm{O}(3,1)}$ covariant form as

$$T_\alpha v^\alpha \psi = 0; \quad (77)$$

similarly, Eqs. (54) and (55) may be recast as

$$T_\alpha v^\alpha \psi_1 = 0. \quad (78)$$

Therefore a hyperspinor is invariant under translation in the direction v^α determined by that hyperspinor.

Consider the quantities defined by

$$x_1^\alpha = (1/4N)\tilde{\psi}\Gamma^4\Gamma^\alpha\Gamma^7\psi_1; \quad (79)$$

using Eqs. (52)–(55) one verifies that

$$v_\alpha x_1^\alpha = 0. \quad (80)$$

Under translation,

$$x_1^\alpha \to T_b x_1^\alpha = (1/4N)\tilde{\psi}\Gamma^4\Gamma^\alpha\Gamma^7(\psi_1 + b^\mu T_\mu \psi) = x_1^\alpha - b^\beta(\delta^\alpha_\beta + v^\alpha v_\beta). \quad (81)$$

In particular, $v_\alpha T_b x_1^\alpha = 0$.

In order to construct the spacetime coordinates x^α of the particle described by the hyperspinor (ψ,ψ_1), we must now introduce a real parameter σ into the formalism. σ is to transform as a scalar under $\overline{\mathrm{SO}(3,1)}$ and inhomogeneously under translation as follows:

$$\sigma \to T_b \sigma = \sigma + b \cdot v. \quad (82)$$

Can σ be constructed from (ψ,ψ_1)? Assume for the moment that $\sigma = \sigma(\psi,\psi_1)$, and moreover that σ is functionally invariant under translation; then $T_b\sigma = \sigma(T_b\psi, T_b\psi_1) = \sigma(\psi, \psi_1 + b^\alpha T_\alpha \psi) = \sigma(\psi,\psi_1) + b \cdot v$. Operating on this expression with $|v^\alpha \partial/\partial b^\alpha|_{b=0}$ yields $(\partial\sigma/\partial\psi_1) T_\alpha v^\alpha \psi = -1$; using Eq. (77), this says $0 = -1$. We conclude that a Lorentz scalar function of (ψ,ψ_1) which is functionally invariant under translation and has the desired translation transformation law of Eq. (82) does not exist. σ may therefore be regarded as representing an independent degree of freedom within this formalism.

Define the (nondimensionalized) coordinates $x^\alpha(p)$, $p \in M_4$, of the particle described by the hyperspinor (ψ,ψ_1) and σ by

$$x^\alpha = \sigma v^\alpha + x_1^\alpha \quad (83)$$

$$= -(1/4N)\tilde{\psi}\Gamma^4\Gamma^\alpha(\sigma\psi - \Gamma^7\psi_1). \quad (84)$$

Under translation

$$x^\alpha \to T_b x^\alpha = (T_b\sigma)v^\alpha + T_b x_1^\alpha = x^\alpha - b^\alpha \quad (85)$$

by Eqs. (81) and (82).

Let m be a parameter with the dimensions of mass. The dimensional position r^α, momentum p^α, and angular momentum $J^{\alpha\beta}$ of the *free* massive magnetic dipole particle described by (ψ,ψ_1) and σ are defined according to

$$r^\alpha = (m^{-1})x^\alpha, \quad (86)$$

$$p^\alpha = m(-g)^{1/2} e^\alpha_{(4)} = mN(-g)^{1/2} v^\alpha, \quad (87)$$

and

$$J^{\alpha\beta} = \Sigma^{\alpha\beta} + r^\alpha p^\beta - r^\beta p^\alpha. \quad (88)$$

Using

$$r^\alpha p^\beta - r^\beta p^\alpha = \tfrac{1}{4}(-g)^{1/2}(-\tilde{\lambda}\gamma^4[S^{\alpha\beta},\gamma_\mu]\lambda_1 + \tilde{\xi}[S^{\alpha\beta},\gamma_\mu]\gamma^4\xi_1)v^\mu, \quad (89)$$

$$= -\tfrac{1}{2}(-g)^{1/2}(\tilde{\xi}\gamma^5 S^{\alpha\beta}\lambda_1 + \tilde{\xi}_1\gamma^5 S^{\alpha\beta}\lambda),$$

$$= \tfrac{1}{2}(-g)^{1/2}\tilde{\psi}\Gamma^4 M^{\alpha\beta}\psi_1, \quad (90)$$

$J^{\alpha\beta}$ may also be expressed as

$$J^{\alpha\beta} = \tfrac{1}{2}[\tilde{\xi}S^{\alpha\beta}(\lambda - (-g)^{1/2}\gamma^5\lambda_1) + (\tilde{\xi} - (-g)^{1/2}\tilde{\xi}_1\gamma^5)S^{\alpha\beta}\lambda]. \quad (91)$$

$\Sigma^{\alpha\beta}$ and p^α satisfy[3]

$$\tfrac{1}{2}\Sigma_{\alpha\beta}\Sigma^{\alpha\beta} = N^2, \quad (92)$$

$$p_\alpha p^\alpha = g m^2 N^2, \quad (93)$$

and

$$v^\alpha \Sigma_{\alpha\beta} = 0 \text{ (Frenkel condition)}. \quad (94)$$

We turn now to the problem of finding equations of motion for the hyperspinor (ψ,ψ_1) and σ that yield, say, the Lorentz force law for the momentum. In this search we are guided by two consistency conditions: any proposed equations of motion must give (i) $\dot{x}^\alpha = dx^\alpha/ds = v^\alpha$ identically (since $v^\alpha v_\alpha = -1$, the parameter s is the nondimensionalized arc length); (ii) $\dot{\xi}_1 = \epsilon\dot{v}\lambda_1 + \epsilon v\dot{\lambda}_1$. Let $E_{\alpha\beta} = -E_{\beta\alpha}$ be some given function of (ψ,ψ_1) and σ. Then, as is straightforward to verify, the following equations of motion ensure that these two consitency conditions are satisfied:

$$\dot{\psi} = -\tfrac{1}{2}E_{\alpha\beta}M^{\alpha\beta}\psi, \quad (95)$$

$$\dot{\psi}_1 = -\tfrac{1}{2}E_{\alpha\beta}M^{\alpha\beta}\psi_1 - 2x^\alpha E_{\alpha\beta}M^\beta{}_\mu\Gamma^7\psi v^\mu, \quad (96)$$

and

$$\dot{\sigma} = 1 - E_{\alpha\beta}x^{\alpha}v^{\beta}. \tag{97}$$

In four-component form,

$$\dot{\lambda} = -\tfrac{1}{2}E_{\alpha\beta}S^{\alpha\beta}\lambda, \tag{98}$$

$$\dot{\xi} = \tfrac{1}{2}E_{\alpha\beta}\tilde{S}^{\alpha\beta}\xi, \tag{99}$$

$$\dot{\lambda}_1 = -\tfrac{1}{2}E_{\alpha\beta}[S^{\alpha\beta}\lambda_1 + 2v^{\mu}(x^{\alpha}S^{\beta}{}_{\mu} - x^{\beta}S^{\alpha}{}_{\mu})\lambda], \tag{100}$$

and

$$\dot{\xi}_1 = \tfrac{1}{2}E_{\alpha\beta}[\tilde{S}^{\alpha\beta}\xi_1 - 2v^{\mu}(x^{\alpha}\tilde{S}^{\beta}{}_{\mu} - x^{\beta}\tilde{S}^{\alpha}{}_{\mu})\xi]. \tag{101}$$

Upon differentiating the definitions of $x^{\alpha}, e^{\alpha}{}_{(\mu)}, \Sigma^{\alpha\beta}$, and N, and then substituting from Eqs. (95)–(101), one finds that

$$\dot{x}^{\alpha} = v^{\alpha}, \tag{102}$$

$$\dot{N} = 0, \tag{103}$$

$$\dot{e}^{\alpha}{}_{(\mu)} = E^{\alpha}{}_{\beta}e^{\beta}{}_{(\mu)} \tag{104}$$

and

$$\dot{\Sigma}^{\alpha\beta} = E^{\alpha}{}_{\mu}\Sigma^{\mu\beta} - E^{\beta}{}_{\mu}\Sigma^{\mu\alpha}. \tag{105}$$

Also

$$(d/ds)\tilde{\xi}\lambda = 0, \tag{106}$$

and utilizing

$$\dot{v} = [-\tfrac{1}{2}E_{\alpha\beta}S^{\alpha\beta}, v], \tag{107}$$

one can easily show that these equations of motion preserve Eqs. (54) and (55):

$$\dot{\xi}_1 = \epsilon\dot{v}\lambda_1 + \epsilon v\dot{\lambda}_1 \tag{108}$$

and

$$\dot{\lambda}_1 = \dot{v}\epsilon\xi_1 + v\epsilon\dot{\xi}_1. \tag{109}$$

Substituting the particular choice

$$E_{\alpha\beta} = (ge/2M)F_{\alpha\beta} + (1 - g/2)(e/M)v^{\mu}(v_{\alpha}F_{\beta\mu} - v_{\beta}F_{\alpha\mu}), \tag{110}$$

where $M = m|N|$ and g is a parameter such that $g - 2$ is a measure of the anomalous magnetic moment of the particle) into Eq. (104) yields the Lorentz force law for p^{α} and the BMT equation for the $e^{\alpha}{}_{(j)}$; in particular this yields the BMT equation for the Pauli–Lubanski pseudovector, which is $e^{\alpha}{}_{(3)}$.[2,3] Here it is to be understood that $F_{\alpha\beta}$ is some prescribed function of (ψ,ψ_1) and σ that describes external electromagnetic fields. This choice for $E_{\alpha\beta}$ should not be taken too seriously; it is meant only to illustrate the existence of a nontrivial self-consistent dynamical scheme for (ψ,ψ_1) and σ. Hopefully it will prove possible to find a minimally constrained Lagrangian whose associated Euler–Lagrange equations for the hyperspinor (ψ,ψ_1) and σ are some variant of Eqs. (95)–(97), and which also yields field equations for $E_{\alpha\beta}[(\psi,\psi_1),\sigma]$.

One last remark. It is possible to bring SU(N) internal degrees of freedom into this classical model with only slight modifications of the formalism. Let ϕ_A $A,B = 1,...,n$ transform under an n-dimensional irreducible representation of SU(N), and $T_{jAB} = T^{*}_{jBA}$ $j,h,k = 1,...,N^2 - 1$ be the infinitesimal generators of this representation of SU(N). The T_j may be normalized according to

$$\mathrm{tr}T_jT_k = 2\delta_{jk} \tag{111}$$

and satisfy

$$[T_j,T_k] = ic_{jkh}T_h, \tag{112}$$

where c_{jkh} is real and totally antisymmetric in $\{j,k,h\}$. Let $\psi^a a,b = 1,...8$ denote the components of ψ and define

$$\psi^a_A = \psi^a\phi_A \tag{113}$$

and define ψ_{1A}, λ_A, and ξ_A similarly. A "gauged" classical observable (constructed from $\psi^a_A, \psi^a_{1A},...$) is denoted by placing a caret over the corresponding ungauged quantity. These classical observables are defined as previously, with the additional stipulation that one is to take the trace over SU(N) indices. Thus, for example, the gauged tetrad is $\hat{e}^{\alpha}{}_{(\mu)} = e^{\alpha}{}_{(\mu)}\phi^{\dagger}\phi$. Note that $\hat{x}^{\alpha} = x^{\alpha}$ and $\hat{v}^{\alpha} = v^{\alpha}$. The gauged equations of motion are

$$\dot{\psi}^a_A = -\tfrac{1}{2}E^j{}_{\alpha\beta}M^{\alpha\beta a}{}_b\psi^b T_{jAB}\phi_B, \tag{114}$$

$$\dot{\psi}^a_{1A} = -\tfrac{1}{2}E^j{}_{\alpha\beta}M^{\alpha\beta a}{}_b\psi^b_1 T_{jAB}\phi_B - 2\hat{x}^{\alpha}E^j{}_{\alpha\beta}M^{\beta}{}_{\mu}{}^{a}{}_{b}\Gamma^{7b}{}_c\psi^c\hat{v}^{\mu}T_{jAB}\phi_B, \tag{115}$$

and

$$\dot{\sigma} = 1 - E^j{}_{\alpha\beta}\phi^{\dagger}T_j\phi\hat{x}^{\alpha}\hat{v}^{\beta}(\phi^{\dagger}\phi)^{-1}, \tag{116}$$

and yield results analogous to Eqs. (102)–(109) (here $E^j{}_{\alpha\beta}$ represents an externally prescribed Yang–Mills field). For example $\dot{\hat{e}}^{\alpha}{}_{(\mu)} = \hat{E}^{\alpha}{}_{\beta}\hat{e}^{\beta}{}_{(\mu)}$, where $\hat{E}_{\alpha\beta} = E^j{}_{\alpha\beta}(\phi^{\dagger}T_j\phi)/(\phi^{\dagger}\phi)$. As with Eqs. (95)–(97), it is important to find a Lagrangian that gives these equations of notion, along with field equations for $E^j{}_{\alpha\beta}$, which utilizes a minimum number of Lagrange multipliers.

Note added to discussion:

In the course of solving the equations of motion (95), (96), and (97) for a few simple cases it became apparent that

$$\psi_1 = -\Gamma_{\alpha}\psi x^{\alpha}_1 \tag{117}$$

is a sort of "first integral" of the equations of motion. Substituting for x^{α}_1 from Eq. (79) into Eq. (117) yields an identity if and only if

$$\tilde{\xi}\lambda_1 = 0. \tag{118}$$

In arriving at this result we have used the identity

$$\gamma_0\tilde{\xi}\gamma^5\lambda + \gamma^5\tilde{\xi}\lambda = \lambda\tilde{\xi}\gamma^5 + \gamma^5\lambda\tilde{\xi} + \epsilon\xi\tilde{\lambda}\gamma^4 - \gamma^4\xi\tilde{\lambda}\epsilon, \tag{119}$$

which may be verified by choosing a representation of the γ matrices and evaluating Eq. (119). Since $(d/ds)\tilde{\xi}\lambda_1 = 0$ and $T_b(\tilde{\xi}\lambda_1) = \tilde{\xi}\lambda_1$. we append to the definition of hyperspinor given by Eqs. (37), (38), (54), and (55) the additional stipulation that Eq. (118) also hold. Hence a hyperspinor possesses ten independent components; together with σ they form a set of possessing eleven independent components.

[1]A. Quadir, J. Math. Phys. 21, 514 (1980).
[2]P. L. Nash, J. Math. Phys. 21, 2534 (1980).
[3]P. L. Nash, J. Math. Phys. 21, 1024 (1980).
[4]Greek indices run from 1 to 4. The metric tensor on M_4 has components $g_{\alpha\beta} = \mathrm{diag}(1,1,1,-1)$ in a Cartesian coordinate system. ϵ_{ABCDEF} is the completely antisymmetric Levi–Civita tensor of weight -1 in six dimensions; $\epsilon_{123456} = +1.\epsilon_{\alpha\beta\mu\nu} = \epsilon_{\alpha\beta\mu\nu 56}\cdot g = \det(g_{\alpha\beta})$.
[5]This definition of Ω differs by a minus sign from that used in Refs. 2 and 3.

Geometrical spacetime perturbation theory: Regular higher order structures

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A coordinate-independent formulation of spacetime perturbation-theory is extended beyond the first-order. Higher-order analogs of the second fundamental form (first metric variation) and corresponding higher-order projection identities lead to higher-order perturbation equations for the spacetime metric fields coupled to spacetime. A deformation-geometrical vertex functional or Frechet derivative is introduced and used to express deformation-covariant perturbation equations in terms of action functionals. The deformation-covariant vertex functionals of the Einstein–Hilbert action functional are computed to fourth order (sufficient for third-order perturbation equations).

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1. INTRODUCTION

Many applications of general relativity reduce to the description of n-parameter families of spacetimes. It is a great advantage to describe such spacetime families in a purely geometrical way which does not depend on a choice of spacetime coordinates or a choice of one member of a family as a "background spacetime." This paper is the second of a series that develops such a description. The previous paper introduced the basic geometrical structures that such a description requires.[1] This paper defines the additional structures that are needed to apply this coordinate-independent approach to spacetime perturbations of arbitrary order.

The main innovation in the previous paper was the use of a particularly convenient deformation connection for taking variational derivatives. The deformation concept itself and the idea of using surface embedding theory to do perturbation theory are not new and have been proposed by others in a variety of contexts.[2]

A full introduction to the geometrical concepts which underlie the calculations in this paper is best obtained by reading the previous paper. However, for easy reference, I have collected a brief summary of notation and results in Sec. 2 of this paper. Section 3 introduces the higher order metric variations and shows that they obey projection identities similar to those satisfied by the first metric variation or second fundamental form. Section 4 discusses the gauge conditions which these higher metric variations satisfy when the Hilbert gauge is imposed on an entire spacetime deformation. Action principles for spactime deformations are introduced in Sec. 5 and used to define deformation-covariant Frechet derivatives or vertex functionals. These vertex functionals are computed to fourth order in Sec. 6.

2. NOTATION AND PREVIOUS RESULTS

This paper uses index notation for all tensors. The corresponding intrinsic notation may be found in the previous paper. Lower case Latin indices range from 0 to $n+3$. Greek indices range from 0 to 3. Upper case Latin indices in parentheses range from 1 to n. An additional index (*) is used to denote components which are associated with an additional perturbation parameter $x(*)$. Semicolons denoted spacetime-covariant derivatives as usual while dots denote deformation-covariant derivatives.

The names of Symbols:

Deformation tensor components	γ^{ab}
Component a of deformation one-form A	$\theta^{(A)}{}_a$
Coordinate a of a deformation chart	x^a
Coordinate (A) of a deformation chart	$x^{(A)} = x^{A+3}$
Spacetime Coordinates of a deformation chart	x^α
Gauge tensor components	$H^a{}_b$
Spacetime curvature tensor components	${}^gR^k{}_{cab}$

A $4+n$ *deformation* consists of a $4+n$ manifold which supports a symmetric *deformation tensor* and a set of n *deformation one-forms* which obey the degeneracy requirements

$$\gamma^{ab}\theta^{(A)}{}_b = 0. \tag{2.1}$$

On such a deformation, one may choose a *gauge* tensor which satisfies:

$$H^a{}_b H^b{}_c = H^a{}_c, \tag{2.2}$$

$$H^a{}_b\theta^{(A)}{}_a = 0, \tag{2.3}$$

$$H^a{}_b\gamma^{bc} = \gamma^{ac}. \tag{2.4}$$

A related object, the *identification gauge* is defined by

$$\iota^a{}_b := \delta^a{}_b - H^a{}_b. \tag{2.5}$$

A coordinate chart $\{x^a\}$ is *aligned* with the gauge H if, in terms of the corresponding coordinate basis, the only nonzero components of H are

$$H^\alpha{}_\beta = \delta^\alpha{}_\beta. \tag{2.6}$$

In an aligned chart, the coordinates $x^{(A)}$ are called *perturbation parameters* and their level-surfaces are the *integral surfaces* of the deformation tensor. The remaining coordinates are *spacetime coordinates* and their level-surfaces are called *identification surfaces.* The only nonzero aligned components of the deformation tensor are the contravariant spacetimes metric tensor components

$$\gamma^{\mu\nu}(x^\alpha,x^{(A)}) = g^{\mu\nu}(x^\alpha,x^{(A)}). \tag{2.7}$$

When these components describe a metric with Lorentz signature, then the deformation is called a *spacetime* $4+n$ *deformation* and the integral surfaces of the deformation tensor are called *spacetimes*.

Once a connection has been chosen on a deformation, the deformation covariant derivative of a vector-field V^a is given by

$$V^a{}_{\cdot b} = V^a{}_{,b} + V^r\Gamma^a{}_{rb}. \tag{2.8}$$

If a gauge H has also been chosen, then one constructs the *second fundamental tensor*

$$h^a{}_{br} := H^a{}_k H^k{}_{r\cdot s} H^s{}_b = H^a{}_{r\cdot s} H^s{}_b. \tag{2.9}$$

A connection is *deformation-compatible* if it satisfies

$$\gamma^{ab}{}_{\cdot c} = 0 \text{ and } \theta^{(A)}{}_{s\cdot c} = 0. \tag{2.10}$$

With a deformation-compatible connection, the second fundamental tensor satisfies the projection identities:

$$h^a{}_{bs} H^s{}_r = 0, \tag{2.11}$$

$$H^a{}_s h^s{}_{br} = h^a{}_{sr} H^s{}_b = h^a{}_{br}. \tag{2.12}$$

A deformation-compatible connection will be called *standard* with respect to the gauge H if it is torsion free (symmetric), renders the identification surfaces flat, and the tensor

$$h^{ab}{}_r := h^a{}_{sr}\gamma^{sb} \tag{2.13}$$

has the symmetry

$$h^{ab}{}_r = h^{ba}{}_r. \tag{2.14}$$

In an aligned chart, a standard deformation connection is characterized by the expressions:

$$h^{\mu\nu}{}_{(A)} = \tfrac{1}{2}\gamma^{\mu\nu}{}_{,(A)}, \tag{2.15}$$

$$\Gamma^{(A)}{}_{bc} = 0, \quad \Gamma^a{}_{(B)(C)} = 0, \tag{2.16}$$

$$\Gamma^\alpha{}_{\beta(C)} = \Gamma^\alpha{}_{(C)\beta} = -h^\alpha{}_{\beta(C)}, \tag{2.17}$$

$$\Gamma^\alpha{}_{\beta\gamma} = \tfrac{1}{2}\gamma^{\alpha\rho}(g_{\rho\beta,\gamma} + g_{\rho\gamma,\beta} + g_{\beta\gamma,\rho}). \tag{2.18}$$

Please notice the factor of one-half in Eq. (2.15). This factor is not standard in gravitational perturbation theory. It was chosen to simplify the deformation geometrical identities. Thus, the vertex functionals which are given in this paper will differ from the standard expressions by powers of two.

The curvature of a deformation connection is defined so that the Ricci identity takes the form

$$V^a{}_{\cdot cb} = V^a{}_{\cdot bc} + V^r R^a{}_{rbc}. \tag{2.19}$$

The Riemann tensor then obeys the usual Bianchi identities. The deformation Ricci tensor is defined by

$$R_{ab} := R^s{}_{asb}, \tag{2.20}$$

and the deformation scalar curvature by

$$R := \gamma^{ab}R_{ab}. \tag{2.21}$$

The previous paper showed that the deformation curvature decomposes as follows:

$$\iota^k{}_s R^s{}_{cab} = \iota^r{}_a \iota^s{}_b \iota^t{}_c R^k{}_{trs} = 0, \tag{2.22}$$

$$H^r{}_a H^s{}_b H^t{}_c R^k{}_{trs} = {}^gR^k{}_{cab}, \tag{2.23}$$

$$H^r{}_a H^s{}_b \iota^t{}_c R^k{}_{trs} = H^r{}_a H^s{}_b (h^k{}_{rc\cdot s} - h^k{}_{sc\cdot r}), \tag{2.24}$$

$$H^r{}_a \iota^s{}_b \iota^t{}_c R^k{}_{trs} = H^r{}_a \iota^s{}_b h^k{}_{rc\cdot s} - h^k{}_{jc} h^j{}_{ab}, \tag{2.25}$$

$$H^r{}_a \iota^s{}_b R^{kc}{}_{rs} = h^k{}_{ab}{}^{\cdot c} - h^c{}_{ab}{}^{\cdot k}. \tag{2.26}$$

3. HIGHER-ORDER FUNDAMENTAL TENSORS OF A SPACETIME

It can be seen from Eqs. (2.7) and (2.15) that the second fundamental tensor expresses the first-order rate of change of the spacetime metric within a family of spacetimes. Thus, it is reasonable to refer to the second fundamental tensor as the *first metric variation*. This alternative name for the second fundamental form calls up new associations[3] and makes it obvious that the *second metric variation tensor* of a spacetime in a $4+n$ deformation ought to be defined by

$$h^a{}_{bcd} := h^a{}_{bc\cdot s}\iota^s{}_d. \tag{3.1}$$

The previous paper showed (Eq. (4.16) in that paper[1]) that this tensor has an unexpected symmetry

$$h^a{}_{bcd} = h^a{}_{bdc}, \tag{3.2}$$

and is related to second derivatives of the spacetime metric in an aligned chart according to

$$h^\delta{}_{\alpha(A)(B)} = \tfrac{1}{2}g^{\delta\rho}{}_{,(A)(B)}g_{\rho\alpha} - h^\delta{}_{\rho(A)}h^\rho{}_{\alpha(B)} - h^\delta{}_{\rho(B)}h^\rho{}_{\alpha(A)}. \tag{3.3}$$

A simple computation using Eqs. (2.9), (2.11), and (2.12) shows that this tensor obeys projection identities similar to those obeyed by the first metric variation (Eqs. (2.11), (2.12)):

$$H^a{}_r h^r{}_{bcd} = H^s{}_b h^a{}_{scd} = \iota^s{}_c h^a{}_{bsd} = \iota^s{}_d h^a{}_{bcs} = h^a{}_{bcd}. \tag{3.4}$$

Now carry the procedure one step further and define the *third metric variation tensor* to be

$$h^a{}_{bcde} := h^a{}_{bc(r\cdot s)}\iota^r{}_d\iota^s{}_e, \tag{3.5}$$

where parentheses indicate symmetrization. Use the projection identities to show that this tensor is a second derivative of the first variation:

$$h^a{}_{bcde} = h^a{}_{bc\cdot(rs)}\iota^r{}_d\iota^s{}_e. \tag{3.6}$$

In this form it is evident that the symmetrization has the effect of reducing the number of independent components that need to be considered. The antisymmetric part that has been discarded consists entirely of terms constructed from the first variation. An application of the lower-order projection identities shows that the third metric variation also obeys a set of projection identities

$$H^a{}_r h^r{}_{bcde} = H^s{}_b h^a{}_{scde} = \iota^s{}_c h^a{}_{bsde} = h^a{}_{bcde}. \tag{3.7}$$

In addition, it has the symmetries

$$h^a{}_{b(cde)} = h^a{}_{bcde} \quad h^{(ab)}{}_{cde} = h^{ab}{}_{cde}. \tag{3.8}$$

Beyond the third metric variation, the rules of the game stay the same. For N greater than or equal to 3, the *Nth metric variation tensor* of a spacetime in a $4+n$ deformation is related to the $(N-1)$th metric variation tensor by

$$h^a{}_{bc\ldots de} := h^a{}_{bc\ldots(r\cdot s)}\iota^r{}_d\iota^s{}_e, \tag{3.9}$$

and to the $(N-2)$th metric variation by

$$h^{a}{}_{bc\ldots jde} = h^{a}{}_{bc\ldots j\cdot(rs)} t^{r}{}_{d} t^{s}{}_{e}. \tag{3.10}$$

By induction, all of these metric variation tensors can be shown to obey the analogs of the projection identities (Eq. (3.7)) and to have symmetries analogous to Eqs. (3.8).

4. HIGHER-ORDER GAUGE CONDITIONS

In the previous paper, it was found that the most natural and convenient way to fix the gauge projection tensor H on a deformation is to impose the Hilbert gauge conditions

$$\bar{h}^{a}{}_{bc\cdot a} = 0, \quad \bar{h}^{a}{}_{bc} := h^{a}{}_{bc} - \tfrac{1}{2} H^{a}{}_{b} h^{s}{}_{sc} \tag{4.1}$$

everywhere in the deformation. Because these conditions are imposed everywhere, they imply conditions on the higher-order metric variations. The technique for obtaining these higher-order gauge conditions is just the one that applies to variations of any set of field equations on a deformation. Take a deformation-covariant derivative of the equations, use the Ricci identity to move the new derivative inside of the ones that are already there, project the new derivative using the identification gauge projection tensor, and then use the definitions of the first metric variation (second fundamental form) to bring the projection tensor inside where the projection identities can eliminate it. The resulting condition on the second metric variation can be put into the form

$$q^{ab}{}_{rs\cdot a} = 0, \tag{4.2}$$

where q is defined by

$$q^{ab}{}_{rs} := \bar{h}^{ab}{}_{rs} - \bar{h}^{ab}(r^{h}s) + \tfrac{1}{4}(\bar{h}^{j}{}_{kr}\bar{h}^{k}{}_{js} - \tfrac{1}{2}h_{r}h_{s})\gamma^{ab} \tag{4.3}$$

and the trace-reversed second metric variation is

$$\bar{h}^{ab}{}_{rs} := h^{ab}{}_{rs} - \tfrac{1}{2}\gamma^{ab} h^{j}{}_{jrs}, \tag{4.4}$$

with trace

$$h_{s} := h^{j}{}_{js}. \tag{4.5}$$

The trace-reversed second variation tensor and the divergence-free second variation which is constructed from it obey all of the same symmetries and projection identities as the metric variations. The simplicity of Eq. (4.2) appears to be peculiar to the second-order. I have not been able to obtain comparable formulations of the higher-order Hilbert gauge conditions.

Equation (4.2) is actually quite surprising. If one is given a particular solution to Einstein's equations and is told that it belongs to a spacetime deformation, then Einstein's equations on the other spacetimes in the deformation can be replaced by Eq. (4.1) and a manifestly hyperbolic system of equations for the second fundamental tensor on each spacetime.[1] Equation (4.1) then plays the role of the initial value equations. The significance of Eq. (4.2) is that, to second-order, the initial value problem remains linear. An initial data set for a second-order perturbation expansion around the given solution to Einstein's equations is specified by a first-order metric variation satisfying Eq. (4.1) and a divergenceless second-order variation tensor satisfying Eq. (4.2). In an aligned frame, these equations are

$$\bar{h}^{\alpha\beta}{}_{(C);\beta} = 0, \quad q^{\alpha\beta}{}_{(R)(S);\alpha} = 0$$

and are thus completely linear. Given any two solutions to the second-order initial value equtions, one can produce many more by linear superposition. To second-order, the evident nonlinearity of Eq. (4.1) is taken care of by the strictly algebraic redefinition of fields given by Eq. (4.3).

A simple way to produce a set of initial conditions that satisfy Eq. (4.1) to arbitrary order is to choose all metric variations higher than the first to be zero. The evolution equations then preserve this initial solution, but with higher-order terms which grow in time. This solution to the deformation initial-value problem yields the usual forms of spacetime perturbation theory.

5. DEFORMATION ACTION PRINCIPLES

The use of action principles in perturbation theory is simply a matter of efficiency. It is a way to incorporate the reciprocity principle and thus reduce the number of separate interaction terms that need to be calculated. It is also a way to make contact with the Hamiltonian canonical formalism.

On a spacetime deformation, an action can be regarded as a function whose value at the point P in the deformation is given by an integral

$$I(P) = \int_{\Sigma_P} {}^{4}\sigma L, \tag{5.1}$$

where

$\Sigma_P =$ the spacetime through the point P,

${}^{4}\sigma =$ the invariant spacetime volume element on Σ_P,

and L is the Lagrangian scalar function. The action principle requires that I be extremal on that part of a deformation which satisfies the field equations.

To obtain the field equations everywhere on a given deformation M, perform the following sequence of steps: Imbed M in a larger deformation M^*. Choose a vector-field V on M^* so that V is nowhere tangent to M. Observe that the covariant derivative of the function I with respect to V is a linear functional of the second fundamental form h_V and the covariant derivatives of any other fields that occur in the Lagrangian so that the extremal condition takes the form

$$\nabla_V I(h_V, \nabla_{V\phi}) = 0 \tag{5.2}$$

of a linear functional. Because the larger deformation was arbitrary, except for its inclusion of M, the arguments of this linear functional are arbitrary tensors so that Eq. (5.2) requires the vanishing of a tensor-distribution on spacetime. Equation (5.2) is the weak form of the field equations.

In order to evaluate expressions such as Eq. (5.2), one needs a way to deal with functionals which are given in terms of spacetime integrals. Let K be a function on a deformation and define the new function F by

$$F(P) := \int_{\Sigma_P} {}^{4}\sigma K.$$

Notice that F is constant on each spacetime so that

$$\nabla_V F = \nabla_{\iota V} F.$$

In terms of aligned chart components,

$$\nabla_V F = V^{(A)} F_{\cdot(A)} = V^{(A)} F_{,(A)}$$

so that

$$\nabla_V F = V^{(A)} \int_{\Sigma_P} {}^4\sigma(K_{\cdot(A)} - Kh^a{}_{a(A)}). \tag{5.3}$$

As an example of the deformation-covariant procedure for obtaining field equations, let L be the scalar curvature and obtain Einstein's vacuum field equations. The fully contracted deformation Bianchi identity

$$R^a{}_{ra} - \tfrac{1}{2}R_{,r} = 0$$

yields the scalar curvature variation immediately:

$$R_{\cdot(A)} = 2\iota^r{}_{(A)} R^a{}_{ra}.$$

Now use this result in Eq. (5.3) and Eq. (5.2) to obtain the vacuum field equations in the form

$$V^{(A)} \int_\Sigma {}^4\sigma(2\iota^r{}_{(A)} R^a{}_{ra} - Rh^a{}_{a(A)}) = 0. \tag{5.4}$$

Convert the total divergence

$$(\iota^r{}_{(A)} R^a{}_r)_{\cdot a} = R^a{}_{(A);a}$$

into a surface integral so that Eq. (5.4) becomes

$$2V^{(A)} \int_{\partial\Sigma} \sigma_\alpha R^\alpha{}_{(A)} - V^{(A)} \int_\Sigma {}^4\sigma(2R^a{}_r \iota^r{}_{(A)\cdot a} + Rh^a{}_{a(A)}) = 0$$

or

$$2V^{(A)} \int_{\partial\Sigma} \sigma_\alpha R^\alpha{}_{(A)} + 2V^{(A)} \int_\Sigma {}^4\sigma(R^a{}_r - \tfrac{1}{2}RH^a{}_r)h^r{}_{a(A)} = 0. \tag{5.5}$$

In particular, let $x^{(*)}$ be an aligned coordinate which is constant on the given deformation M and choose V to have $V^{(*)} = 1$ as its only nonzero component. Equation (5.5) then requires

$$\int_{\partial\Sigma} \sigma_\alpha R^\alpha{}_{(*)} + \int_\Sigma {}^4\sigma G^a{}_r h^r{}_{a(*)} = 0. \tag{5.6}$$

The surface term can be discarded by imposing boundary conditions on the larger deformation M^*. If the larger deformation is otherwise arbitrary, then so is the tensor field $h^r{}_{a(*)}$ and Eq. (5.6) is the weak form of Einstein's equations.

The field equations which are obeyed by metric and field perturbations may also be obtained from the action. The equations which determine the evolution of the second fundamental form or first metric variation $h^a{}_{bc}$ within each spacetime of a deformation are just

$$I_{\cdot(C)(*)}[h^r{}_{a(*)}, \phi_{\cdot(*)}, h^r{}_{a(C)(*)}, \phi_{\cdot(C)(*)}] = 0, \tag{5.7}$$

and the second metric variation $h^a{}_{bcd}$ obeys the system

$$I_{\cdot((C)(D)(*))} = 0. \tag{5.8}$$

Notice that Eq. (5.7) has two sets of arbitrary arguments and therefore gives two sets of field equations. One set is the desired first-order system while the other is just a repetition of the zero-order field equations already given by Eq. (5.6). Equation (5.8) has an even larger variety of arbitrary arguments and yields the zero- and first-order field equations several times over in addition to the desired second-order equations. This wasteful repetition of the lower-order equations can be avoided by defining a deformation-covariant Frechet derivative (sometimes called the vertex function).[4]

Let F be a deformation functional of the sort that appears in Eq. (5.3) and define the functional

$$\nabla F[(\gamma,\phi):\Sigma_P]\cdot(h_{e_{(A)}}, \nabla_{e_{(A)}}\phi) := \nabla_{e_{(A)}} F[(\gamma,\phi):\Sigma].$$

It is convenient to suppress the arguments and use the abbreviation

$$(f_{(A)}) := (h_{e_{(A)}}, \nabla_{e_{(A)}}\phi) \tag{5.9}$$

for the entire collection of field variations. Thus, the definition becomes

$$\nabla F\cdot(f_{(A)}) := F_{\cdot(A)}(f_{(A)}). \tag{5.10}$$

This functional is simply an abbreviated form of the ordinary gradient of F on the deformation. It is also the covariant first Frechet derivative.

Now define a new functional, the covariant second Frechet derivative, by

$$\nabla^2 F := F_{\cdot(A)(B)} - \tfrac{1}{2}\nabla F\cdot(\nabla_{e_{(A)}} f_{B}) - \tfrac{1}{2}\nabla F\cdot(\nabla_{e_{(B)}} f_{(A)}).$$

Because of vanishing torsion in the first term and linearity in the last two terms, the second field variations occur only in the symmetric combination

$$f_{(A)(B)} := \tfrac{1}{2}\nabla_{e_{(A)}} f_{(B)} + \tfrac{1}{2}\nabla_{e_{(B)}} f_{(A)} \tag{5.11}$$

or

$$f_{(A)(B)} = \{h^\rho{}_{\sigma(A)(B)}, \phi_{\cdot((A)(B))}\}.$$

Because of the familiar chain-rule for noncovariant Frechet derivatives[4] these symmetric combinations of second derivatives all cancel so that the resulting functional is independent of second variations. Thus, the covariant second Frechet derivative takes the form

$$\nabla^2 F\cdot(f_{(A)}, f_{(B)}) := F_{\cdot(A)(B)} - \nabla F\cdot(f_{(A)(B)}). \tag{5.12}$$

The use of deformation-covariant derivatives in Eq. (5.12) instead of the partial derivatives which are natural for noncovariant Frechet derivatives does not interfere with the Frechet chain-rule because the connection coefficients simply introduce terms which depend only on first derivatives. The key property of the Frechet type of derivative is the cancellation of higher derivatives and this property is not affected by the use of deformation-covariant derivatives.

Now generalize Eqs. (5.11) and (5.12) by the following recursive definitions:

$$f_{(A)\cdots(B)(C)} := \tfrac{1}{2}\nabla_{e_{(B)}} f_{(A)\cdots(C)} + \tfrac{1}{2}\nabla_{e_{(C)}} f_{(A)\cdots(B)}$$

$$\begin{aligned}\nabla^{r+1}F\cdot(f_{(A)},\ldots,f_{(B)},f_{(C)}) &:= \tfrac{1}{2}[\nabla^r F\cdot(f_{(A)},\ldots,f_{(B)})]_{\cdot(C)} \\ &\quad + \tfrac{1}{2}[\nabla^r F\cdot(f_{(A)},\ldots,f_{(C)})]_{\cdot(B)} \\ &\quad - \tfrac{1}{2}\nabla^r\cdot F(f_{(A)(C)},\ldots,f_{(B)}) - \cdots - \tfrac{1}{2}\nabla^r\cdot F(f_{(A)},\ldots,f_{(B)(C)}) \\ &\quad - \tfrac{1}{2}\nabla^r\cdot F(f_{(A)(B)},\ldots,f_{(C)}) - \cdots \\ &\quad - \tfrac{1}{2}\nabla^r\cdot F(f_{(A)},\ldots,f_{(C)(B)}).\end{aligned} \tag{5.13}$$

Here again, the fact that each of these functionals depends only on the first-field variations follows from the Frechet derivative chain-rule which governs the highest-order variations at each recursion. The symmetrization which guarantees that each of these covariant Frechet derivatives is symmetric in all of its first-variation arguments has no effect on the highest derivative terms because these are already symmetric.[4]

In terms of the covariant Frechet derivatives defined by Equations (5.9)–(5.13), the field equations which an action I induces on a deformation M are

$$\nabla I(\gamma,\phi)\cdot(f_{(*)}) = 0, \tag{5.14}$$

$$\nabla I(\gamma,\phi)\cdot(f_{(A)(*)}) + \nabla^2 I(\gamma,\phi)\cdot(f_{(A)},f_{(*)}) = 0, \tag{5.15}$$

$$\begin{aligned}\nabla I(\gamma,\phi)\cdot(f_{(A)(B)(*)}) &+ \nabla^2 I(\gamma,\phi)\cdot(f_{(A)(B)},f_{(*)})\\ &+ \nabla^2 I(\gamma,\phi)\cdot(f_{(A)},f_{(B)(*)})\\ &+ \nabla^3 I(\gamma,\phi)\cdot(f_{(A)},f_{(B)},f_{(*)}) = 0,\end{aligned} \tag{5.16}$$

and so on. Each of these equations requires a distribution to vanish because the variations $f_{(*)}$, $f_{(A)(*)}$, $f_{(A)(B)(*)}$ in the "extra direction" are arbitrary collections of tensor fields. At each order, the field equations can be simplified by using the lower-order equations. Thus, when Eq. (5.14) is satisfied, Eq. (5.15) becomes

$$\nabla^2 I(\gamma,\phi)\cdot(f_{(A)},f_{(*)}) = 0 \quad \text{for all } f_{(*)}, \tag{5.17}$$

while Eq. (5.16) simplifies to just

$$\nabla^2 I(\gamma,\phi)\cdot(f_{(A)(B)},f_{(*)}) + \nabla^3 I(\gamma,\phi)\cdot(f_{(A)},f_{(B)},f_{(*)}) = 0. \tag{5.18}$$

Thus Eq. (5.17) governs the first variation $f_{(A)}$ which drives the second variation through Eq. (5.18). Further deformation-covariant derivatives and use of the lower-order equations yield still higher-order equations. For example, the third-order field variations (or third-order perturbations) are governed by the system

$$\begin{aligned}\nabla^2 I\cdot(f_{(A)(B)(C)},f_{(*)}) &+ \nabla^3 I\cdot(f_{(A)(B)},f_{(C)},f_{(*)})\\ &+ \nabla^3 I\cdot(f_{(A)(C)},f_{(B)},f_{(*)}) + \nabla^3 I\cdot(f_{(A)},f_{(B)(C)},f_{(*)})\\ &+ \nabla^4 I\cdot(f_{(A)},f_{(B)},f_{(C)},f_{(*)}) = 0.\end{aligned}$$

The combinatorial logic of the equations which govern higher-order field variations is transparent and lends itself to the same diagram notation as the usual approach to perturbation theory with each covariant Frechet derivative of the action represented by a vertex.[5] Because of this diagram notation, the functional $\nabla^r I$ will be called a *deformation-covariant vertex functional of order r*.

6. THE CALCULATION OF VERTEX FUNCTIONALS

Once the deformation-covariant vertex functionals have been obtained, perturbation theory proceeds as it always has. However, these vertex functionals are not the usual Frechet derivatives and *the resulting perturbation theory has undergone a nontrivial rearrangement of orders.* Furthermore, the techniques for calculating the vertex functionals are entirely new. In order to demonstrate these techniques, I will calculate the first three deformation-covariant vertex functionals of the Hilbert gravitational action functional

$$I_g = \frac{1}{16\pi}\int {}^4\sigma R.$$

For simplicity, I will discard all surface terms and use the Hilbert gauge condition throughout.

The first-order vertex functional follows from the calculation that led to Eq. (5.6) and is just

$$\nabla I_g\cdot(f_{(*)}) = \frac{1}{8\pi}\int {}^4\sigma G^a{}_r h_{ra(*)}. \tag{6.1}$$

This particular expression does not assume the Hilbert gauge condition. Thus, one is free to consider a deformation M^* in which the Hilbert gauge metric variation vanishes but the metric variation h does not. In such a case, there is a tensor-field a on M^* whose only nonzero aligned chart components are $a^a(*)$ and the metric variation is

$$h^{ra}{}_{(*)} = -a^{(r}{}_{(*)}{}^{;a)}. \tag{6.2}$$

A deformation of this type does not alter spacetimes at all so that the variation of the action I must vanish. The resulting identity is

$$0 = \int {}^4\sigma(G_{rs}H^s{}_a)a^{(r}{}_{(*)}{}^{;a)}. \tag{6.3}$$

This identity yields the Bianchi identities.

For higher-order vertex functions, one can repeat the argument that led to Eq. (6.3) and conclude that all vertex functionals vanish when one of their linear arguments is a purely longitudinal variation such as the one described by Eq. (6.2). Once this essential fact has been realized, there is no longer any need to consider longitudinal variations and one might as well impose the Hilbert gauge once and for all.

This sort of gauge specialization has been frowned upon in the past. In the usual approach to perturbation theory, a gauge condition is an infinitesimal coordinate condition and necessarily breaks general covariance. Here, there is no connection between gauge and coordinate conditions (unless one insists upon aligned coordinates). Thus, imposing the Hilbert gauge here is no worse than imposing the Lorentz gauge in electrodynamics.

The second-order vertex function is obtained by taking the deformation-covariant derivative of the first-order vertex functional, projecting it along a direction aligned with the gauge, and ignoring all terms that have second metric variations. Thus, I obtain

$$\begin{aligned}\nabla^2 I_g\cdot(f_{(A)},f_{(*)}) &= [\nabla I\cdot(f_{(*)})]_{,s}\iota^s{}_{(A)}\text{-second variations}\\ &= \frac{1}{8\pi}\int {}^4\sigma\{G^a{}_{r,s}\iota^s{}_{(A)}h^r{}_{a(*)} - G^a{}_r h^r{}_{a(*)}h^j{}_{j(A)}\}.\end{aligned}$$

The previous paper used the deformation Bianchi and Gauss–Codazzi identities and the Hilbert gauge conditions to compute

$$\begin{aligned}G^{ar}{}_{,s}\iota^s{}_{(A)}\\ = \bar{h}^{ar}{}_{(A)}{}^{;k}{}_{k} + 2[R^a{}_k{}^r{}_t - \tfrac{1}{2}\gamma^{ar}R_{kt}]\bar{h}^{kt} + G^{ar}h^j{}_{j(A)}.\end{aligned}$$

With this result, the second-order vertex function becomes

$$\begin{aligned}\nabla^2 I\cdot(f_{(A)},f_{(*)}) = (1/8\pi)\int {}^4\sigma\{h^r{}_{a(*)}\bar{h}^a{}_{r(A)}{}^{;k}{}_k\\ + 2h^r{}_{a(*)}[R^a{}_{krt} - \tfrac{1}{2}H^a{}_r R_{kt}]\bar{h}^{kt}{}_{(A)}\}.\end{aligned} \tag{6.4}$$

The computation of still higher vertex functionals can be reduced to a mechanical routine if one notices that appropriate integrations by parts can be used to express all vertex functionals in terms of just three tensors:

$$h^{a}{}_{bc}, \quad h^{a}{}_{bc\cdot d}, \quad \text{and} \quad R^{a}{}_{b}{}^{c}{}_{d}.$$

The $h^{a}{}_{bc}$ factors are of no consequence because differentiating them yields second variations which are subtracted in the final expression for the vertex functions. For the remaining two tensors, the Ricci identity, the Codazzi identity, and the definition of h yield

$$\begin{aligned}
h^{ab}{}_{(A)\cdot}{}^{k}{}_{s}\iota^{s}{}_{(B)} &= h^{ab}{}_{(A)\cdot s}{}^{k}\iota^{s}{}_{(B)} + h^{rb}{}_{(A)}R^{a}{}_{rs}{}^{k}\iota^{s}{}_{(B)} \\
&\quad - h^{a}{}_{r(A)}R^{rb}{}_{s}{}^{k}\iota^{s}{}_{(B)} \\
&= (h^{ab}{}_{(A)\cdot s}\iota^{s}{}_{(B)})^{\cdot k} + h^{ab}{}_{(A)\cdot s}h^{sk}{}_{(B)} \\
&\quad - h^{rb}{}_{(A)}(h^{ak}{}_{(B)\cdot r} - h_{r}{}^{k}{}_{(B)}{}^{\cdot a}) \\
&\quad + h^{a}{}_{r(A)}(h^{rk}{}_{(B)\cdot}{}^{b} - h^{bk}{}_{(B)}{}^{\cdot r}) \\
&= h^{ab}{}_{(A)(B)}{}^{\cdot k} + h^{ab}{}_{(A)\cdot s}h^{sk}{}_{(B)} + h^{b}{}_{r(A)}h^{rk}{}_{(B)}{}^{\cdot a} \\
&\quad + h^{a}{}_{r(A)}h^{rk}{}_{(B)}{}^{\cdot b} \\
&\quad - h^{a}{}_{r(A)}h^{bk}{}_{(B)}{}^{\cdot r} - h^{b}{}_{r(A)}h^{ak}{}_{(B)}{}^{\cdot r},
\end{aligned} \tag{6.5}$$

and the deformation Bianchi identities yield the relation

$$\begin{aligned}
R^{abcd}{}_{\cdot s}\iota^{s}{}_{(B)} &= -R^{abd}{}_{s}{}^{\cdot c}\iota^{s}{}_{(B)} - R^{ab}{}_{s}{}^{c\cdot d}\iota^{s}{}_{(B)} \\
&= -(R^{abd}{}_{(B)})^{\cdot c} - R^{abd}{}_{s}h^{sc}{}_{(B)} + (R^{abc}{}_{(B)})^{\cdot d} \\
&\quad + R^{abc}{}_{s}h^{sd}{}_{(B)}.
\end{aligned} \tag{6.6}$$

When a curvature factor appears in a spacetime integral, one integrates the derivatives in Eq. (6.6) by parts and obtains the operator identity

$$\begin{aligned}
R^{abcd}{}_{\cdot s}\iota^{s}{}_{(B)} &= R^{abd}{}_{(B)}\nabla^{c} - R^{abc}{}_{(B)}\nabla^{d} + R^{abc}{}_{s}h^{sd}{}_{(B)} \\
&\quad - R^{abd}{}_{s}h^{sc}{}_{(B)},
\end{aligned}$$

where the derivatives are understood to act on all of the other factors in a given term. The Codazzi equation then expresses the result of differentiating and projecting the curvature factor:

$$\begin{aligned}
&R^{abcd}{}_{\cdot s}\iota^{s}{}_{(B)} \\
&\quad = (h^{ad}{}_{(B)}{}^{\cdot b} - h^{bd}{}_{(B)}{}^{\cdot a})\nabla^{c} - (h^{ac}{}_{(B)}{}^{\cdot b} - h^{bc}{}_{(B)}{}^{\cdot a})\nabla^{d} \\
&\quad + R^{abc}{}_{s}h^{sd}{}_{(B)} - R^{abd}{}_{s}h^{sc}{}_{(B)}.
\end{aligned} \tag{6.7}$$

Notice that, just as was promised at the beginning of this paragraph, Eqs. (6.5) and (6.7) involve no new tensors and show that all of the vertex functionals can be expressed in terms of the tensors h, ∇h, and $\mathbf{R}$.

Equations (6.5) and (6.7) provide a straightforward way to perform the derivatives called for by Eqs. (5.3) and (5.13). The reader who is familiar with the variational procedure for computing vertex functionals will recognize that Eqs. (6.5) and (6.7) are essentially the usual expressions for varying the connection and curvature.[6] Where, then, is the computational advantage of the deformation-covariant approach? It lies in the fact that one can raise and lower tensor indices at will without ever worrying about variations of the spacetime metric tensor. All of the annoying terms that usually arise from the variation of metric tensor factors have been absorbed into the deformation-covariant derivatives. Thus, one obtains expressions which are shorter and more comprehensible than the usual ones. Because there are only three tensors involved and there is no need to worry about which indices are up and which are down, a simple diagram notation can be used for all of the vertex function calculations.

I find an index-diagram notation to be an indispensable tool for dealing with very high-rank tensors that have many contractions. However, such notations are simply substitution codes for ordinary tensor analysis and have no content of their own. Thus, I will not burden the reader with my own personal code and leave him to develop his own.

The deformation-covariant third order vertex functional is fairly simple to calculate and is short enough to be included here:

$$\begin{aligned}
\nabla^{3}I_{g} = (1/16\pi)\int {}^{4}\sigma\,\mathrm{Sym}\{ &-12h^{a}{}_{b(A)\cdot r}h^{rs}{}_{(B)}h^{b}{}_{a(*)\cdot s} \\
&+ 24h^{a}{}_{b(A)\cdot r}h^{r}{}_{s(B)}h^{s}{}_{a(*)}{}^{\cdot b} + 8R^{a}{}_{b}h^{b}{}_{c(A)}h^{c}{}_{d(B)}h^{d}{}_{a(*)} \\
&- 12h_{(A)}h^{r}{}_{s(B)}R^{s}{}_{ar}{}^{b}h^{a}{}_{b(*)} + 6h_{(A)}h_{(B)}R^{a}{}_{b}h^{b}{}_{a(*)} \\
&- 3h_{(A)}h_{(B)}{}^{\cdot r}h_{(*)\cdot r} + 2h_{(A)}h^{a}{}_{b(B)\cdot s}h^{b}{}_{a(*)}{}^{\cdot s} \\
&- h_{(A)}h_{(B)}h_{(*)}R\},
\end{aligned} \tag{6.8}$$

where Sym denotes a symmetrization on all of the indexes in parentheses—on (A), (B), and $(*)$. The Hilbert gauge condition and the Ricci identity have been used to simplify this expression somewhat. However, the lower-order field equations have not been used and it is fairly easy to see that they would produce substantial additional simplification. If, in addition, one is perturbing a spacetime in which the first-order equations preserve the trace conditions $h_{(A)} = 0$, then only the first two terms of Eq. (6.8) survive and one sees the lowest-order graviton-scattering vertex function for the simple object that it is.

The deformation-covariant fourth-order vertex functional is also simple to calculate. With an efficient diagram notation, it is an afternoon's work. I find 22 terms, not counting symmetrization, and do not find the result very illuminating. However, there are uses for third-order perturbation theory and the deformation-covariant form of the interaction term is simpler than the usual one. On the chance that someone will derive an insight from one or more of its 22 terms, I include my result for the fourth-order vertex in the appendix.

The computation of still higher-order deformation-covariant vertex functionals of the Hilbert action is straightforward, but increasingly tedious if one insists on keeping all of the terms. However, vertex functionals for special types of deformations can be calculated to much higher-orders without much trouble. For example, if one only cares about deformations with $h_{(A)} = 0$, then one can make this specialization right at the start without making any error. The fourth-order vertex then reduces to eight terms and the fifth-order vertex is obtainable without too much effort—it has somewhat less than 55 terms (depending on how many of them turn out to involve $h_{(A)}$) before like terms are combined.

The relatively compact form of Eq. (6.8) is not simply a trick of notation. If all of the deformation-covariant derivatives are expressed in terms of spacetime-covariant derivatives, only eight new terms result and these all vanish by the projection identities. Thus, one can just replace dots by semicolons everywhere in Eq. (6.8).

Do these deformation-covariant techniques really save effort? I believe that they do as much as any formal technique can be expected to do. For the calculation of variational derivatives and high-order field equations, they lead one to make useful forms of the perturbation equations. For example, the first-order perturbation equations for the gravitational field are obtained in just the form that Sciama and Gilman found by trial and error to be the most advantageous one.[7] It is always possible to argue that an intelligent and alert theoretician would make the proper groupings of terms without this formalism. However, it is surely easier to use a formalism which produces efficient calculations without effort. Furthermore, once one goes beyond fourth-and fifth-order calculations, one is almost certainly in the realm of computer-assisted algebra. For such calculations one must use a formalism that supplies intelligent groupings of terms automatically.

7. CONCLUSIONS

Two geometrical structures are needed to formulate higher-order spacetime perturbations in a coordinate-independent way: the higher-order metric variation tensors and the deformation-covariant vertex functionals of a given action. The process of computing the first four gravitational vertex functionals in this deformation-covariant way has revealed two basic advantages: (1) The calculations are entirely straightforward and mechanical with no penalties for arranging indices and terms in the wrong way; (2) the Hilbert gauge, with its enormous simplification of the gravitational interaction, can be imposed without restricting spacetime coordinates. The first advantage is a mere convenience but a powerful one when computers are used to do the algebra. The second advantage is potentially useful because it allows one to choose coordinates that are comoving with matter while retaining the simplicity of the Hilbert gauge for gravitational waves. Even when there is no matter around, the fact that the gauge condition does not restrict spacetime coordinates means that one is still free to impose such conditions as $h^{0\mu}{}_{(A)} = 0$ in order to fix the coordinates. The resulting coordinates are, of course, not aligned with the gauge, but the fact that all of the objects that one has to deal with are deformation tensors makes this misalignment a minor inconvenience.

In order to make the nature of deformation geometry as clear as possible I have deliberately chosen the most time-honored (i.e., old-fashioned) and universal way to do differential geometry. More powerful approaches to differential geometry in general and the computation of curvature tensors in particular are available. The calculus of differential forms and the various offshoots of the Newman–Penrose formalism are some well-known examples of such powerful computational techniques. Because the deformation-covariant approach to perturbation theory is only a slight variation on standard Riemannian geometry, there is nothing to prevent any of these powerful techniques from being used to do deformation-covariant perturbation theory.

APPENDIX: THE FOURTH ORDER DEFORMATION- COVARIANT GRAVITATIONAL VERTEX FUNCTIONAL IN THE HILBERT GAUGE

$$\begin{aligned}
\nabla^4 I_g = (1/16\pi)\int^4 \sigma\,\mathrm{Sym}\,\{ & -24h^{a}{}_{b(A)\cdot r}h^{r}{}_{s(B)}h^{s}{}_{k(C)}h^{b}{}_{a(*)}{}^{\cdot k} + 72h^{a}{}_{b(A)\cdot r}h^{r}{}_{s(B)}h^{b}{}_{k(*)}h^{s}{}_{a(C)}{}^{\cdot k} \\
& -24h^{a}{}_{b(A)\cdot r}h^{r}{}_{s(B)}h^{k}{}_{a(*)}h^{s}{}_{k(C)}{}^{\cdot b} + 24h^{a}{}_{b(A)\cdot r}h^{s}{}_{a(B)}h^{k}{}_{s(*)}h^{r}{}_{k(C)}{}^{\cdot b} + 16h^{a}{}_{b(A)\cdot r}h^{r}{}_{a(B)}h^{b}{}_{s(*)}h^{s}{}_{r(C)}{}^{\cdot r} \\
& -24h^{a}{}_{b(A)\cdot r}h^{r}{}_{s(B)}h^{b}{}_{k(*)}h^{k}{}_{a(C)}{}^{\cdot s} - 16h^{a}{}_{b(A)\cdot r}h^{b}{}_{k(B)}h^{k}{}_{s(*)}h^{s}{}_{a(C)}{}^{\cdot r} + 16R^{a}{}_{db}{}^{c}h^{b}{}_{a(A)}h^{d}{}_{s(C)}h^{s}{}_{r(*)}h^{r}{}_{c(B)} \\
& -24h_{(B)}R^{a}{}_{db}{}^{c}h^{b}{}_{a(A)}h^{d}{}_{s(C)}h^{s}{}_{c(*)} - 12h_{(A)}h_{(B)\cdot r}h^{r}{}_{s(C)\cdot k}h^{ks}{}_{(*)} - 24h_{(B)\cdot r}h^{r}{}_{s(A)}h^{s}{}_{j(C)\cdot k}h^{kj}{}_{(*)} \\
& -56h_{(A)}h^{a}{}_{b(B)\cdot r}h^{b}{}_{s(*)}h^{r}{}_{a(C)}{}^{\cdot s} + 40h_{(A)}h^{a}{}_{b(B)\cdot r}h^{r}{}_{s(*)}h^{b}{}_{a(C)}{}^{\cdot s} + 24h^{a}{}_{b(A)}h^{b}{}_{a(B)\cdot r}h^{r}{}_{s(*)}h_{(C)}{}^{\cdot c} \\
& +24h_{(A)}h_{(B)}R^{a}{}_{db}{}^{c}h^{b}{}_{a(*)}h^{d}{}_{c(C)} - 8h_{(A)}h_{(B)}h^{a}{}_{b(*)\cdot r}h^{b}{}_{a(C)}{}^{\cdot r} - 6h_{(A)}h_{(B)\cdot r}h^{r}{}_{s(*)}h_{(C)}{}^{\cdot s} \\
& +8h_{(A)}h^{a}{}_{b(B)\cdot r}h^{s}{}_{a(*)}h^{r}{}_{s(C)}{}^{\cdot b} - 8h_{(A)}h_{(B)}h_{(C)}R^{a}{}_{b}h^{b}{}_{a(*)} + 6h_{(A)}h_{(B)}h_{(C)\cdot r}h_{(*)}{}^{\cdot r} \\
& -4h_{(A)}R^{a}{}_{b}h^{b}{}_{c(B)}h^{c}{}_{d(C)}h^{d}{}_{a(*)} + h_{(A)}h_{(B)}h_{(C)}h_{(*)}R\,\}. \qquad \text{(A1)}
\end{aligned}$$

[1] R. H. Gowdy, J. Math. Phys. **19**, 2294–304 (1978).

[2] R. Geroch, Commun. Math. Phys. **13**, 180–93 (1969); J. M. Stewart and M. Walker, Proc. R. Soc. London A **341**, 49–74 (1974); R. E. Kates, "Underlying Structure of Singular Perturbations on Manifolds," Smithsonian Observatory Center for Astrophysics Preprint Series No. 1269 (1979).

[3] Note that the term "third fundamental form" cannot be used for the next higher-order object because it traditionally means the matrix square of the second fundamental form. N. J. Hicks, *Notes of Differential Geometry* (Van Nostrand, New York, 1965).

[4] The Frechet derivative of a functional F of the spacetime

$$DF(g_{\mu\nu})\cdot(\delta g_{\mu\nu}) := \partial F(g_{\mu\nu} + \epsilon\delta g_{\mu\nu})/\partial\epsilon.$$

For a more formal treatment, see S. Lang, *Differential Manifolds* (Addison-Wesley, Reading, Massachusetts, 1972).

[5] Each classical correlation function

$$\langle\langle (A)(B)\cdots(*)\rangle\rangle := \int {}^4\sigma h^{a}{}_{b(A)(B)\cdots}h^{b}{}_{a(*)}$$

can be expressed as a sum of tree diagrams. See, for example, B. S. DeWitt, *Relativity, Groups, and Topology*, edited by C. DeWitt and B. DeWitt (Gordon and Breach, New York, 1964), esp. p. 773. In the classical expression, internal lines represent Green's functions which are usually retarded and external lines represent first-order field variations such as $h^{a}{}_{b(A)}$.

[6] *Ibid.*, p. 716; C. W. Misner, K. S. Thorne, and J. A. Wheeler, *Gravitation* (Freeman, San Francisco, 1973), p. 967.

[7] D. W. Sciama, P. C. Waylen, and R. C. Gilman, Phys. Rev. **187**, 1762–6 (1969).

Note on Finslerian relativity

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Finslerian structure of spacetime is investigated. For a special type of generalized Finsler metric the explicit expression of Cartan-like metrical connection is derived and it is shown that it resembles the usual one. Causal problems in Finsler-type spacetime are discussed and, based on the arguments, the Einstein-type equations for the Finslerian quantities are derived by using the lifting of a Finsler metric to a tangent bundle. It is shown that a solution of the proposed equations can also be obtained from the complex structure of the tangent bundle. One-form type metrics are used to discuss the geometrical interpretation of isosymmetry. A simple way of obtaining a metrical connection for a general generalized Finsler metric is given.

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1. INTRODUCTION

P. Finsler founded a new geometry (nowadays it is called the Finsler geometry) in 1918 in his dissertation.[1] It is a generalization of the Riemannian geometry in some sense. After that many mathematicians investigated such a geometry (see, e.g., Cartan[2]), though there are not many applications of the geometry to physical problems. An overall review was given by Ingarden.[3] We shall review some of the applications of the geometry.

After Yukawa developed his bilocal theory,[4] several authors investigated the Finslerian aspect of the theory. In Yukawa's bilocal theory, physical quantities depend on the pair of events (x_1^i, x_2^i) or equivalently on the center-of-mass coordinate (x^i) and the relative coordinate (r^i). On physical grounds, we may set the condition

$$r^i r_i = \lambda^2 \quad (\lambda = \text{const}),$$

and hence the quantities in Yukawa's theory depend on (x^i) and the *direction* of (r^i). Such a pair is usually called the line element and the set of all line elements forms precisely an underlying manifold of the Finsler geometry. Therefore it is expected that the Finsler geometry plays a fundamental role in Yukawas's bilocal theory (trilocal or multilocal theory can also be expressed by using the Finsler-type geometry). Based on this aspect several authors (see, e.g. Ref. 5) formulated Yukawa's theory using the Finsler (or Finsler-type) geometry.

Apart from Yukawa's theory, Finsler geometry plays some roles in particle physics. In Finsler geometry an indicatrix $\{y|L(x,y)=1\}\subset M_x$, which is a three-dimensional hypersurface in a tangent space, plays a very important role. Horváth[6] investigated the symmetry group of an indicatrix and showed that it may be interpreted as the isosymmetry group, and he classified the elementary particles according to this symmetry group of the indicatrix. Several years ago Drechsler developed the geometrical theory of gauge theory.[7] His theory is constructed over the de Sitter bundle and it is, roughly speaking, a spacetime whose tangent spaces are the curved Riemannian spaces (de Sitter spaces). Finsler geometry has precisely the same interpretations because it can be interpreted as the union of the curved tangent spaces M_x which are equipped with the Riemannian metric $g_{ij}(x, y)$ (x being fixed). In this repect the tangent bundle, which is the union of all tangent spaces at all points of spacetime, must play an important role in gauge theory. Actually it can be shown[8] that the extremal curve in a tangent bundle may be considered as the path of a particle with internal degrees of freedom in curved spacetime.

In another branch of physics, relativity, Randers (and others[9]) investigated the special type of Finsler metric of the form

$$ds = \{g_{ij}(x)dx^i dx^j\}^{1/2} + k_i dx^i.$$

the extremal curves of ds are, as is well known, the paths of charged point particles in the Riemmanian spacetime which is equipped with the metric tensor $g_{ij}(x)$. Randers discussed the relations of these metrics to the five-dimensional relativity of Kalza and Klein.[10] The above type of metric ds was originally investigated by Weyl.[11] However, Einstein pointed out the nonintegrability of length transfer, which implies that spectral frequencies of lines emitted by atoms depend on their histories. This inconvenience is, however, circumvented by the recent work by Sen *et al.*,[12] i.e., by using the modified Weyl geometry, called the Lyra geometry. Horváth[13] proposed the further-developed theory based on a general fundamental function $ds = L(x^i, \dot{x}^i)dt$. One of his field equations is the generalization of the Lorentz equation

$$A_{ijk} = -\tfrac{1}{2}(S_{ij|k} + S_{jk|i} + S_{ki|j}), \tag{1.1}$$

where

$$A_{ijk} = L(x, \dot{x})C_{ijk}$$

and C_{ijk} is a v-torsion tensor of the Finsler space (see Sec. 2); S_{ij} is a symmetrized stress-energy tensor. By contracting j and k in Eq. (1), we have

$$A_i = -\partial S_i{}^k/\partial x^k,$$

which is just the density of the Lorentz force of the field. Eq. (1) determines the y-dependence of the metric tensor $g_{ij}(x, y)$. For this point Takano[14] proposed another type of equation. His equations are

$$S_{ij} - \tfrac{1}{2}g_{ij}S = -\kappa T^{(\mathrm{int})}_{ij},$$

where S_{ij}, S are v-Ricci curvature tensor, v-scalar curvature, respectively, and $T^{(\mathrm{int})}_{ij}$ is the internal energy–momentum tensor. In Sec. 4 we shall give another type of equation which determine x and y dependence of $g_{ij}(x, y)$.

Interesting papers have been published concerning the application of the Finsler geometry to high energy cosmic ray physics.[15] Asanov,[12] especially, developed the generalized Einstein equation based on a special type of Finsler metric (Berwald-Moór type Finsler metrics).

Further, the following application of the Finsler geometry seems to be possible. According to the theorem proven by Penrose and Hawking,[16] it is becoming clear that the big bang singularity of our universe about ten billion years ago is inevitable (at least classical-theoretically) if we accept the several physically reasonable conditions (e.g., the positiveness of the energy). Then the following problem arises naturally. Is the big bang singularity inevitable even if the quantum effects are taken into account? However, before considering the quantum effects, the following approach seems to be interesting. As was shown by Horváth,[5] Yukawa's nonlocal theory can be described by the Finsler-type geometry and it seems nautral to consider that, near the big band, the universe is highly condensed and thus it may be considered as a giant elementary particle. Therfore, the universe may be described by the Finsler-type geometry. Now if we accept this possibility, we have to investigate the causal structure in Finsler-type spacetime.[17] We shall discuss this point in Sec. 3. Since the underlying manifold of the Finsler geometry is a tangent bundle, it is quite reasonable to investigate the structure of the tangent bundle. In Sec. 4 we shall investigate such problems.

The style of this note is the following: In Sec. 2 a brief summary of the concepts of the Finsler geometry is given. However, the method in this section is slightly more general than the usual one, i.e., we shall obtain a Cartan-like connection for the slightly generalized Finsler-type metrics. In Sec. 3 the causal problem of the Finsler-type metrics is discussed in connection with physical grounds. Section 4 is devoted to the lifted Riemannian metrics in the tangent bundle and also a new Einstein-type equation is presented. Section 5 is devoted to the complex manifold structure of the tangent bundle. It seems interesting to consider a tangent bundle as a complex manifold. Section 6 contains concluding remarks. In the appendices problems concerning the generalized Finsler metrics are discussed. Also the relation between the 1-form type Finsler metrics and the isosymmetry is discussed.

2. FINSLER GEOMETRY

We begin our discussion of the Finsler geometry by giveing a "model" of Finsler space by quoting the sentences from the letter of P. Finsler to M. Matsumoto. We believe that the model helps us to imagine what Finsler spaces are.

In der Astronomie misst man die Entfernungen gerne in einem Zeitmass, insbesondere in Lichtjahren. Nimmt man 1 Sekunde als Einheit, dann sind die Einheitsflächen Kugeln mit einem Radius von 300,000 *km. Zu jedem Punkt im Raum gehört eine solche Einfernungen und damit die Geometrie im Raum, im einfachsten Fall die euklidische. Wenn aber die Lichtstrahlen als "kürzeste Linine" in Gravitationsfeldern gekrümmt verlaufen, wird man eine Riemannsche Geometrie erhalten. Ebenso kann in anisotropen Medien die Lichtgeschwindigkeit von der Richtung abhängen, die Einheitsflächen sind dann keine Kugeln mehr. Nun misst man auch im Gelände auf der Erdoberfläche die Entfernungen oft in einem Zeitmass, etwa in Gehminuten (so die Angaben auf Wegzergern). Die Einheitskurven (für* 1 *minute als Einheit) können allgemeine Kurven sein, auch ohne Mittelpunkt (da man in* 1 *Minute aufwärts weiniger weit kommt als abwärts); sie definieren eine "allgemeine Geometrie," die ein wohl nicht sehr exaktes, aber doch anschauliches "Modell" darstellt. Die "kürzesten Linien", auf denen man am schnellsten zum Ziel kommt (etwa zu einer Bergspitze), können kompliziert verlaufen.* [Note: *Allgemeine Geometrie* = Finsler geometry, *Einheitsflächen* = indicatrix.]

The model is illustrated in Fig. 1.

First we explain the concept of the Finsler connection. In Finsler spaces, quantities depend on both the position coordinate (x^i) and the direction vector (y^i). The coordinate transformations are defined by

$$\bar{x}^a = f^a(x), \quad \bar{y}^a = y^j\, \partial\bar{x}^a/\partial x^j, \tag{2.1}$$

and thus if there exist the quantities $N^k{}_i(x, y)$ which transform, under the coordinate transformation (2.1), according to the rule

$$y^j \frac{\partial^2 \bar{x}^a}{\partial x^j \partial x^i} = N^k{}_i \frac{\partial \bar{x}^a}{\partial x^k} - \bar{N}^a{}_c \frac{\partial \bar{x}^c}{\partial x^i},$$

we can define a covariant differential operator by

$$\frac{\delta}{\delta x^k} \equiv \frac{\partial}{\partial x^k} - N^i{}_k \frac{\partial}{\partial y^i}. \tag{2.2}$$

When $\delta/\delta x^k$ acts on a scalar function $f(x, y)$, $f_{,k} \equiv \delta f/\delta x^k$ defines the vector quantity.

Next if there exist the quantities $F_i{}^k{}_j$ which transform, under the coordinate transformation (2.1), according to the rule

$$\bar{F}_a{}^c{}_b \frac{\partial x^k}{\partial \bar{x}^c} = F_i{}^k{}_j \frac{\partial x^i}{\partial \bar{x}^a} \frac{\partial x^j}{\partial \bar{x}^b} + \frac{\partial^2 x^k}{\partial \bar{x}^a \partial \bar{x}^b},$$

then, for a vector u^i, the following quantity derived from u^i is the tensor

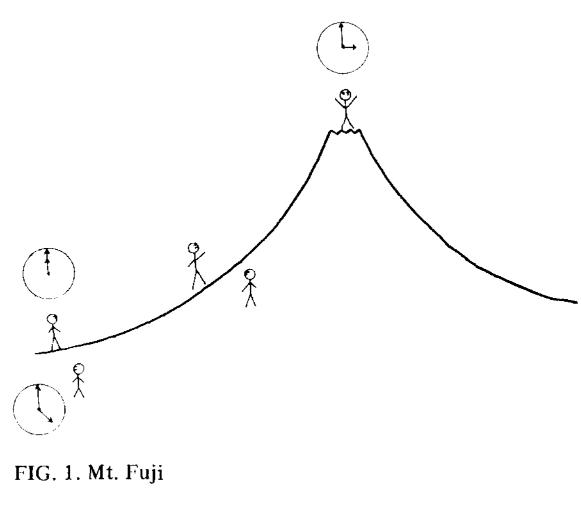

FIG. 1. Mt. Fuji

$$u^i{}_{|j} \equiv \delta u^i/\delta x^j + u^k F_k{}^i{}_j.$$

That is to say, in Finsler spaces, the *pair* $(F_k{}^i{}_j, N^i{}_j)$ defines the covariant derivative with respect to x^k. $N^i{}_j$ are called the *nonlinear connection parameters*.

In a Finsler space we also have the derivative with respect to y^k. From the transformation formulas (2.1), for a given vector u^i, the following quantity is a tensor:

$$u^i{}_{||j} \equiv \partial u^i/\partial y^j.$$

However, more generally, by using the tensor quantities $C_j{}^i{}_k$,

$$u^i|_j \equiv \partial u^i/\partial y^j + u^k C_k{}^i{}_j$$

also define a tensor quantity.

We shall call the triplet $F\Gamma = (F_j{}^i{}_k, N^i{}_k, C_j{}^i{}_k)$ a *Finsler connection*. In the following we shall determine the Finsler connection $F\Gamma$ from a given Finsler-type metric tensor $g_{ij}(x, y)$ by imposing the several conditions of the Finsler connection.

Before determining a Finsler connection $F\Gamma$ we shall explain the Finsler metrics. Assume that we are given a differentiable manifold M which is equipped with a line element $ds = L(x, dx)$. The function $L(x, dx)$ is called the *fundamental function* and should be homogeneous of degree 1 in dx. The Riemannian spaces are the special cases of the Finsler spaces which correspond to the ones being equipped with the following special type of fundamental functions,

$$ds^2 = g_{ij}(x)dx^i dx^j \equiv L^2(x, dx).$$

In this special case the metric tensor of the space is defined by

$$g_{ij}(x) \equiv \frac{1}{2}\frac{\partial^2 L^2}{\partial dx^i \partial dx^j}. \tag{2.3}$$

In Finsler spaces, we define analogously the metric tensor $g_{ij}(x, dx)$, which corresponds to the given fundamental function $L(x, dx)$, by Eq. (2.3). However, in this general case the metric tensor g_{ij} depends on both x and dx. From the homogeneity property of $L(x, dx)$ in dx, from now on we shall use a vector y instead of an infinitesimal vector dx. Thus we may write

$$g_{ij}(x, y) \equiv \frac{1}{2}\frac{\partial^2 L^2(x, y)}{\partial y^i \partial y^j} \equiv LL_{ij} + L_i L_j, \tag{2.4}$$

where the subscript on L denotes defferentiation with respect to y. Usually the Cartan connection is defined by using the metric tensor given by (2.4). Here, however, we shall derive a Cartan-like Finsler connection for a slightly more general Finsler-type metric $g_{ij} \equiv LL_{ij} - \alpha L_i L_j$, where α is a scalar function of x only (the usual Finsler metric corresponds to the case $\alpha = -1$). By imposing the metrical and the torsionless conditions, $F\Gamma$ is determined.[18] In the following we shall set $N^i{}_j$ equal to $y^k F_k{}^i{}_j$.[19] The metrical condition means $g_{ij}|_k = g_{ij|k} = 0$ and the torsionless condition means $C_j{}^i{}_k = C_k{}^i{}_j$, $F_j{}^i{}_k = F_k{}^i{}_j$. From these conditions one can determine $F\Gamma$ as follows: From $g_{ij}|_k = 0$, we get

$$\partial_{(k)} g_{ij} = g_{ir} C_j{}^r{}_k + g_{jr} C_i{}^r{}_k \quad (\partial_{(k)} \equiv \partial/\partial y^k).$$

Paying attention to the relations

$$g_{ij} = \tilde{g}_{ij} - (1+\alpha)L_i L_j, \quad \tilde{g}_{ij} \equiv LL_{ij} + L_i L_j,$$

we have

$$\partial_{(k)}\tilde{g}_{ij} - (1+\alpha)(L_{ik}L_j + L_i L_{jk}) = g_{ir}C_j{}^r{}_k + g_{jr}C_i{}^r{}_k. \tag{2.5}$$

(In the following the quantities with tildes denote the corresponding quantities derived from the Finsler metric $\tilde{g}_{ij}$). From (2.5) we obtain

$$C_i{}^r{}_k = \tilde{C}_i{}^r{}_k + \frac{1+\alpha}{\alpha} l^r L_{ik}, \quad \left(l^r \equiv \frac{y^r}{L}\right).$$

Next we consider the condition $g_{ij|k} = 0F$. From this equation we have $(F_j{}^i{}_k \equiv g^{ir} F_{jrk})$,

$$2\gamma_{ijk} = 2F_{ijk} + N^r{}_k \partial_{(r)} g_{ij} + N^r{}_i \partial_{(r)} g_{jk} - N^r{}_j \partial_{(r)} g_{ik}, \tag{2.6}$$

where

$$2\gamma_{ijk} = \partial_i g_{jk} + \partial_k g_{ij} - \partial_j g_{ik} \quad (\partial_i \equiv \partial/\partial x^i).$$

Multiplying (2.6) by y^i and using the relation $y^i \partial_{(r)} g_{ij} = -(1+\alpha)LL_{jr}$, we have

$$2\gamma_{0jk} = (1-\alpha)N_{jk} + (1+\alpha)N_{kj} - \alpha(1+\alpha) \times (L_j L_r N^r{}_k - L_k L_r N^r{}_j) + N^r{}_0 \partial_{(r)} g_{jk}, \tag{2.7}$$

where the subscript 0 means the contraction with y^i, e.g., $\gamma_{0jk} \equiv y^i \gamma_{ijk}$.[20] From (2.7) we have

$$\gamma_{0jk} + \gamma_{0kj} = N_{jk} + N_{kj} + N^r{}_0 \partial_{(r)} g_{jk}, \tag{2.8}$$

$$\alpha^{-1}(\gamma_{0jk} - \gamma_{0kj}) = N_{kj} - N_{jk} - (1+\alpha) \times (L_j L_r N^r{}_k - L_k L_r N^r{}_j). \tag{2.9}$$

From (2.8) and (2.9) we get

$$2N_{kj} = (1+\alpha^{-1})\gamma_{0jk} + (1-\alpha^{-1})\gamma_{0kj} + (1+\alpha)(L_j L_r N^r{}_k - L_K L_r N^r{}_j) - N^r{}_0 \partial_{(r)} g_{jk}. \tag{2.10}$$

Next multiplying (2.6) by $y^i y^k$ and $y^i y^j$, we obtain

$$\gamma_{0j0} = -\alpha \tilde{g}_{jr} N^r{}_0, \tag{2.11}$$

$$\gamma_{00k} = -\alpha LL_r N^r{}_k, \tag{2.12}$$

respectively. By Eqs. (2.6), (2.10)–(2.12) we can determine F_{ijk} from γ_{ijk}. These formulas reduce to the usual Cartan connection if $\alpha = -1$. The properties of the metric which corresponds to the $\alpha = 1$ case will be discussed in the author's forthcoming paper.[18]

If $\alpha = -1$ we have $(g_{ij} = \tilde{g}_{ij})$,

$$C_i{}^r{}_k = C_i{}^r{}_k,$$

$$2F_{ijk} = 2\gamma_{ijk} - N^r{}_k \partial_{(r)} g_{ij} - N^r{}_i \partial_{(r)} g_{jk} + N^r{}_j \partial_{(r)} g_{ik},$$

$$2N_{kj} = 2\gamma_{0kj} - N^r{}_0 \partial_{(r)} g_{jk},$$

$$N_{j0} = \gamma_{0j0}.$$

In the following we shall develop the Finsler geometry for this special case $\alpha = -1$ (we shall drop the tilde from $\tilde{g}_{ij}$).

In analogy to the Riemannian case, covariant derivatives are defined by

$$K^i{}_{j|k} \equiv \delta K^i{}_j/\delta x^k + K^r{}_j F_r{}^i{}_k - K^i{}_r F_j{}^r{}_k,$$

$$K^i{}_j|_k \equiv \partial K^i{}_j/\partial y^k + K^r{}_j C_r{}^i{}_k - K^i{}_r C_j{}^r{}_k,$$

where [see (2.2)],

$$\frac{\delta}{\delta x^k} \equiv \frac{\partial}{\partial x^k} - N^r{}_k \frac{\partial}{\partial y^r}, \quad N^r{}_k \equiv y^a F_a{}^i{}_k.$$

Corresponding to the Riemannian case, one can obtain the Ricci identities. In the Finslerian case, however, there are three types of Ricci identities. Here we consider only the Cartan connection:

$$u^i{}_{|j|k} - u^i{}_{|k|j} = u^r R_r{}^i{}_{jk} - u^i|_r R^r{}_{jk},$$

$$u^i{}_{|j}|_k - u^i|_{k|j} = u^r P_r{}^i{}_{jk} - u^i{}_{|r} C_j{}^r{}_k - u^i|_r P_j{}^r{}_k,$$

$$u^i|_j|_k - u^i|_k|_j = u^r S_r{}^i{}_{jk}.$$

Curvature parts and torsion parts

The curvatures are given by[21]

$$R_r{}^i{}_{jk} = \mathfrak{S}_{jk}\left\{\frac{\delta F_r{}^i{}_j}{\delta x^k} + F_r{}^s{}_j F_{s\,i\,k}\right\} + C_r{}^i{}_s R^s{}_{jk},$$

$$P_{rijk}(\equiv g_{ia} P_r{}^a{}_{jk}) = \mathfrak{S}_{ri}\{C_{ikj|r} + C_{rja} P_i{}^a{}_k\},$$

$$S_{rijk}(\equiv g_{ia} S_r{}^a{}_{jk}) = \mathfrak{S}_{jk}\{C_{rka} C_i{}^a{}_j\}.$$

The torsions are given by

$$R^i{}_{jk} = R_0{}^i{}_{jk},$$

$$P_j{}^i{}_k = P_0{}^i{}_{jk} = C_j{}^i{}_{k|0} = y^a \frac{\partial F_a{}^i{}_j}{\partial y^k} \quad \text{(see Refs. 14 and 15).}$$

In the Finsler spaces there are many Bianchi identities. For our case the independent Bianchi identities are

$$\mathfrak{S}_{jkl}\{R_h{}^i{}_{jk|l} + P_h{}^i{}_{jr} R^r{}_{kl}\} = 0,$$

$$\mathfrak{S}_{jkl}\{R_j{}^i{}_{kl} - C_j{}^i{}_r R^r{}_{kl}\} = 0,$$

$$\mathfrak{S}_{jk}\{C_k{}^h{}_{i|j} + C_j{}^h{}_r P_k{}^r{}_i - P_j{}^h{}_{ki}\} = 0,$$

$$\mathfrak{S}_{jk}\{R_l{}^h{}_{jr} C_k{}^r{}_i + P_l{}^h{}_{jr} P_k{}^r{}_i + P_l{}^h{}_{ki|j}\} + S_l{}^h{}_{kr} R_{rij} + R_l{}^h{}_{jk}|_i = 0,$$

$$\mathfrak{S}_{jk}\{P_l{}^h{}_{ij}|_k - P_l{}^h{}_{rk} C_i{}^r{}_j - S_l{}^h{}_{rk} P_i{}^r{}_j\} + S_l{}^h{}_{jk|i} = 0,$$

$$\mathfrak{S}_{jkl}\{S_i{}^h{}_{jk}|_l\} = 0.$$

These identities are obtained, taking account of the Ricci identities, by the usual methods.

We conclude this section by giving an example of a special type of Finsler space. [For further details of the special Finsler spaces the reader should consult suitable books (see, e.g., Matsumoto[22])].

The example we give here is the space which is derived from the following fundamental function:

$$L(x, y) = \{y^1 y^2 y^3 y^4\}^{1/4}, (*)$$

or, more generally,

$$L(x, y) = \left\{\prod_{a=1}^{4} [h^a_i(x) y^i]\right\}^{1/4}, (**).$$

The peculiar property of these metrics is the following:

(a) $C_i \equiv C_i{}^j{}_j = 0.$

The metric has the further following properties:

(b) $R_{hijk} = 0, \quad P_{hijk} = 0.$

The properties (a) and (b) will be used in Secs 4 and 5.

The metric (*) is an example of the following locally-Minkowski spaces. The locally-Minkowski spaces are the Finsler spaces whose metric tensors are, if we choose the suitable coordinate system, independent of the space coordinate (x^i). The condition for a given Finsler space with the Cartan connection to be a locally-Minkowski space is, as is well known,

$$R_{hijk} = 0 = C_{hij|k}.$$

3. CAUSAL PROBLEM IN FINSLER SPACES

To see what kind of situations occur in the Finsler-type spaces, we use a special type of generalized Finsler metrics which have some interesting properties.

A usual Finsler metric is the second-rank tensor derived from a fundamental function $L(x, y)$ by the equation $LL_{ij} + L_i L_j$ (see Sec. 2). However this definition, becomes too restrictive in some cases and we have to extend the concepts of the Finsler metrics.[5] Since the most essential point of the Finsler metrics is their dependence on the directional coordinates (y^i), we may call a symmetric tensor $g_{ij}(x, y)$, homogeneous of degree zero in y, a *generalized Finsler metric* (GFM) if it is a nondegenerate tensor. One type of GFM appears naturally in the following theorem:

Theorem: Let $\tilde{g}_{ij}(x, y)$ be a usual Finsler metric and $g_{ij}(x, y)$ be the tensor derived from $\tilde{g}_{ij}(x, y)$ and the unit vector field $n_i(x, y)$, positively-homogeneous of degree 0 in y defined by the equations

$$g_{ij}(x, y) = \tilde{g}_{ij}(x, y) - 2n_i(x, y) n_j(x, y). \quad (3.1)$$

The $g_{ij}(x, y)$ is the usual Finsler metric if and only if the $n_i(x, y)$ are y-independent.

As an example of a GFM we examine the following indefinite metric $g_{ij} = LL_{ij} - L_i L_j$; this metric is the $\alpha = 1$ case discussed in Sec. 2. It is also the GFM derived from a usual Finsler metric by Eq. (3.1) with the choice of $n_i = y_i / L$, and it is an interesting GFM for the following reasons: (a) it is an indefinite tensor; (b) almost all of the properties of the usual Finsler metric $LL_{ij} + L_i L_j$ remain true without or with slight modifications;[18] (c) $L^{-2} g_{ij}$ is conformally invariant[23] (d) Horváth–Moór's[24] methods of obtaining the connection parameters are not applicable.

The observable property of this metric tensor is that every vector X^i is timelike if we define the causality by the condition that $g_{ij}(x, X) X^i X^j$ is negative; however, for a fixed y, $g_{ij}(x, y)$ is the indefinite Riemannian metric tensor. How should we interpret such metrics? It seems that this kind of feature is not peculiar to the GFM but also to the usual indefinite Finsler metrics. We think that, without specifying y, we cannot obtain the physically reasonable causal relations in Finsler (or Finsler-type) spaces.[25] In the following we shall discuss such a problem.

In contrast with the case of the Riemannian metrics, the number of candidates of the lightcone may not be two in Finsler-type metrics. This kind of property was first discussed by Beem[26] and he investigated the causal structure of the two-dimensional Minkowski spaces in great detail. To begin with, we first review his approaches.

Suppose M is a four-dimensional differentiable manifold, and the Finsler metric $g_{ij}(x, y)$ is assumed to have signature $+2$, i.e., for any (x, y) it has three positive eigenvalues and one negative one. Let x_0 be the fixed point and y_0 be the given vector at x_0 such that $L(x_0, y_0) = -1$. Construct a simple convex neighborhood $U(x_0)$ about x_0 by $\{x \in M \mid L(x, y_0) < 0\}$. Let $K_1(x)$ be the connected component of $\{y \mid L(x, y) = -1\}$ that contains ky_0 for some $k > 0$. Next he defined a future lightcone $B(x)$ by $\{\theta y \mid y \in K_1(x), \theta \in R_+\}$. Beem defined the causal relation as follows. For $p, q \in U(x_0)$ define $p < q$ if there is a solution $x(s)$ of the following geodesic equation in $U(x_0)$ [with the initial conditions $x(0) = p$, $x(s_0) = q$ and $x'(0) \in B(p)$]:

$$x^{j''} + \gamma_h{}^j{}_k(x, x')x^{h'}x^{k'} = 0,$$

where $\gamma_h{}^j{}_k$ is the Christoffel symbol of the metric g_{ij} [see (2.6)]. On the basis of these preliminaries he showed that the relation $<$ is actually the partial ordering on M.

The essential point of the Beem's arguments is how to define the directional field (y). Since a metric tensor in the Finsler spaces depends on both the position coordinates and the directional coordinates, the metric tensor has no meaning if we do not specify the directional variable (y). Beem performed this by using the continuity of the fundamental function $L(x, y)$. Though Beem's definition is an attractive one, it has a flaw from the physical point of view (see discussion below).

First of all, if we want to consider the Finsler metrics as a model of the spacetime, fundamental physical experiment is the measurement of spacelike separations by using a lamp and a clock. Before considering the Finslerian case, we first examine the Riemannian case and then proceed to the Finslerian one.

Usually spacelike separations are measured as follows[27]: Let C be a world line of a clock on which we are lying. At the event P we emit a photon to a mirror and at the event B it is reflected by the mirror; then we receive it at the event Q on C. Let τ_1, τ_2 be the proper time intervals between P and A, A and Q, respectively. Then the separation between the events A and B is $c(\tau_1\tau_2)^{1/2}$ ($c =$ velocity of light). This measurement can be performed because the concept of the lightlikeness has already been defined. The lightcone is, here, defined by using the usual Lorentz metric $\eta_{ij} = \mathrm{diag}(-1, 1, 1, 1)$. However, in the case of the Finsler-type spacetime, the metric tensor $g_{ij}(x, y)$ depends on, *even locally*, the directional variables and thus there are two possibilities in defining the causality:

(I) V^i will be called null if $g_{ij}(x, y)V^iV^j = 0$ for some fixed y (relative definition),

(II) V^i will be called null if $g_{ij}(x, V)V^iV^j = 0$ (absolute definition).

Which should we take as the definition of the lightlikeness? Beem took (II) as the definition of light. If we take (I) as the definition of the lightlikeness, the method used above for the Riemannian case is also applicable and we can measure the spacelike separations. However, if we take (II) as the definition of the lightlikeness, it is impossible to measure the spacelike separations by the method used above because, if we apply the method, we can obtain only two equations for the four components l^i as shown below:

$$\tau_1{}^2 g_{ij}(A, \xi)e^ie^j + 2\tau_1 g_{ij}(A, \xi)e^il^j + g_{ij}(A, \xi)l^il^j = 0,$$
$$\tau_2{}^2 g^{ij}(A, \eta)e^ie^j - 2\tau_2 g_{ij}(A, \eta)e^il^j + g_{ij}(A, \eta)l^il^j = 0, \tag{3.2}$$

where e^i, ξ^i, and η^i are the unit vectors in the directions $\overrightarrow{PQ}$, $\overrightarrow{PB}$, and $\overrightarrow{BQ}$, respectively. However, the length $\overline{AB}$ is defined by ($l = \overrightarrow{AB}$ is taken as the element of support)

$$\overline{AB}^{\,2} = g_{ij}(A, l)l^il^j, \tag{3.3}$$

so we cannot determine $\overline{AB}$ from Eqs. (3.2) since the directional arguments of (3.2) and (3.3) are different. The above arguments show the necessity of defining the causal relations by (I). That is, we have to fix an element of support independently of the individual motion of a particle (or a reference system) if we consider the causality relations very seriously (cf. Takano[5]).

Then if we take (I) in defining the causal relations, how should we fix an element of support (y) in $g_{ij}(x, y)$? One easy way is to chose an absolute parallel vector field as y, although this choice of y restricts the base Finsler space because the Finsler spaces with the absolute parallel vector field should have zero h-torsion tensor, i.e., $R^i{}_{jk} = 0$. Though this condition is very restrictive, it attracts us because it is known that in this special Finsler space, we can easily construct the Einstein-type tensor by contracting the Bianchi identity in Finsler space. Here we briefly sketch the construction[14,28].

Let us define the Einstein equation in Finsler space by

$$R^{ij} - \tfrac{1}{2}g^{ij}R = \kappa T^{ij},$$

where R^{ij} is the h-Ricci tensor in the Finsler space and T^{ij} is the energy-momentum tensor. Now by contracting the following Bianchi identity

$$\mathfrak{S}_{jkl}\{R_h{}^i{}_{jk|l} + P_h{}^i{}_{jr}R^r{}_{kl}\} = 0,$$

we have

$$(R^{ij} - \tfrac{1}{2}g^{ij}R)_{|j} = U^i,$$

where

$$U_i = \tfrac{1}{2}g^{am}P_a{}^b{}_{(mn}R^n{}_{bi)}.$$

Hence we get

$$T^{ij}{}_{|j} = (1/\kappa)U^i.$$

If there exists an absolute parallel vector field, then $R^i{}_{jk} = 0$ and hence $U^i = 0$, i.e., the energy–momentum is conserved.[29,30]

Based on the previously given arguments on the photon reflection experiments, henceforth we shall take (I). The next problem is how to choose an element of support (y). There are many ways of choosing an element of support. One way is, as was stated previously, to choose an absolute parallelism as y. Another way is to consider that the quantities in Finsler spaces depend intrinsically on y, e.g., the motion of a particle in Finsler spaces is described by the pair (x, y). This possibility is interesting; however it is difficult to develop the causal relation for such a case because the metric tensor for such a case has two negative eigenvalues.[31] So in this paper we consider only the space with the absolute parallelism as the candidate of spacetime (see, e.g., Horváth[5]). In Finslerian theory the physical quantities depend on both the position coordinate (x) and the directional vector (y). In such theory it is natural to consider that the field equations should be derived from *one* variational principle, i.e., not from two, the equation for x-parts and the one for y-parts. In this respect, it is interesting to investigate a theory in tangent bundles. In the next section we shall investigate such a theory based on the assumption $R^{\,i}_{\ jk} = 0$.

At the end of this section we mention the Asanov's metric. Asanov[15] fixed an element of support by using a tetrad system of the underlying manifold, i.e., he set y^m equal to $h^m(x) = \Sigma_A h^m_A(x)$, where $\{h^m_A(x)\}$ is the tetrad system at x. From a relativistic point of view, we think that we have to determine a tetrad system $\{h^m_A(x)\}$ from some field equations which play the same role as the Einstein equations do in the Riemannian spacetime metric tensor $g_{ij}(x)$ (cf Ref. 32). For this purpose, how about lifting a one-form metric[33] to a tangent bundle? That is to say, how about considering the Einstein equations in the tangent bundle which is equipped with a lifted Riemannian metric? By equating the Ricci tensor in the tangent bundle to zero (i.e., the vacuum case), we have the equations $C_i = 0$ and the differential equations of the cotorsion tensor

$$K^{\,i}_{\ jk} = \tfrac{1}{2}g^{ia}\{g_{ba}T_k{}^b{}_j + g_{jb}T_a{}^b{}_k + g_{kb}T_a{}^b{}_j\}.$$

To solve these equations, we may put the fundamental function $L(x, y)$ into the Asanov type metric (see Sec. 2).

4. LIFTED METRIC AND EINSTEIN TENSOR IN A TANGENT BUNDLE

Lifting of a Riemannian metric to a tangent bundle was originated by Sasaki[34] and the concepts were generalized to the Finslerian case by several authors.[35] We briefly summarize the concepts.

Let $g_{ij}(x, y)$ be a Finsler metric on a manifold M. The lifted metric on a tangent bundle is defined by[36]

$$d\sigma^2 = G_{\alpha\beta}dx^\alpha dx^\beta = g_{ij}dx^i dx^j + g_{ij}Dy^i Dy^j,$$

where

$$Dy^i \equiv dy^i + N^i{}_j dx^j,$$

$$(x^\alpha) = (x^i, y^i) \quad (i, j = 1, ..., n) \quad (\alpha, \beta = 1, ..., 2n),$$

and $N^i{}_j$ are the nonlinear connection parameters (see Sec. 2). We shall also use the indices with the parentheses $(i) = n + i$ (e.g., $x^{(i)} = y^i$). Here, however, instead of calculating the Ricci tensors with respect to the basis $\{\partial/\partial x^\alpha\}$, we shall calculate them with respect to the nonholonomic basis introduced by Yano and Davies.[35] They introduced the following basis in the tangent bundle:

$$X_\alpha = \{X_i, X_{(i)}\},$$

$$X_i = \partial/\partial x^i - N^j{}_i\partial/\partial y^j, \quad X_{(i)} = \partial/\partial y^i.$$

The basis $\{X_\alpha\}$ is the dual basis to the 1-forms $\{dx^i, Dy^i\}$. The components of the metric tensor relative to the basis $\{X_\alpha\}$ are

$$G_{\alpha\beta} = \begin{pmatrix} g_{ij} & 0 \\ 0 & g_{ij} \end{pmatrix}.$$

The basis $\{X_\alpha\}$ do not commute with each other (i.e., are nonholonomic),

$$[X_\alpha, X_\beta] \equiv \Omega_\alpha{}^\gamma{}_\beta X_\gamma.$$

The Riemann–Christoffel symbols are defined by

$$\nabla_{X_\alpha} X_\beta \equiv \Gamma_\alpha{}^\gamma{}_\beta X_\gamma,$$

and by the torsionless condition, these quantities are related to the nonholonomic object $\Omega_\alpha{}^\gamma{}_\beta$ by

$$\Gamma_\alpha{}^\gamma{}_\beta - \Gamma_\beta{}^\gamma{}_\alpha = \Omega_\alpha{}^\gamma{}_\beta.$$

The components of the curvature tensor relative to the nonholonomic basis $\{X_\alpha\}$ are obtained from the following curvature form:

$$R(X, Y)Z = [\nabla_X, \nabla_Y]Z - \nabla_{[X,Y]}Z.$$

By a simple computation we have

$$\bar{R}_\beta{}^\alpha{}_{\delta\gamma} = \mathfrak{S}_{\gamma\delta}\{X_\gamma\Gamma_\delta{}^\alpha{}_\beta + \Gamma_\delta{}^\epsilon{}_\beta\Gamma_\gamma{}^\alpha{}_\epsilon\} - \Omega_\gamma{}^\epsilon{}_\delta\Gamma_\epsilon{}^\alpha{}_\beta,$$

where $\bar{R}_\beta{}^\alpha{}_{\delta\gamma}$ are defined by

$$R(X_\gamma, X_\delta)X_\beta \equiv \bar{R}_\beta{}^\alpha{}_{\delta\gamma}X_\alpha.$$

The Ricci tensor and the scalar curvature are defined by $\bar{R}_{\alpha\beta} \equiv \bar{R}_\alpha{}^\gamma{}_{\beta\gamma}$ and $\bar{R} \equiv G^{\alpha\beta}\bar{R}_{\alpha\beta}$ respectively.

The Christoffel symbols were calculated by Yano and Davies[35] and the results are (here we shall change the notations for those used by Matsumoto[22])

$$\Gamma_j{}^h{}_i = F_j{}^h{}_i,$$

$$\Gamma_{(j)}{}^h{}_i = C_j{}^h{}_i + \tfrac{1}{2}g^{ha}R_{jia},$$

$$\Gamma_j{}^h{}_{(i)} = C_j{}^h{}_i + \tfrac{1}{2}g^{ha}R_{ija},$$

$$\Gamma_{(j)}{}^h{}_{(i)} = P_j{}^h{}_i,$$

$$\Gamma_j{}^{(h)}{}_i = -C_j{}^h{}_i - \tfrac{1}{2}R^{\,h}{}_{ij},$$

$$\Gamma_{(j)}{}^{(h)}{}_i = -P_j{}^h{}_i,$$

$$\Gamma_j{}^{(h)}{}_{(i)} = F_j{}^h{}_i,$$

$$\Gamma_{(j)}{}^{(h)}{}_{(i)} = C_j{}^h{}_i.$$

The nonzero $\Omega_\beta{}^\alpha{}_\gamma$'s are

$$\Omega_i{}^{(r)}{}_j = -R^{\,r}{}_{ji} = -\Omega_j{}^{(r)}{}_i,$$

$$\Omega_i{}^{(r)}{}_{(j)} = F_i{}^r{}_j + P_i{}^r{}_j = -\Omega_{(j)}{}^{(r)}{}_i.$$

Using these Christoffel symbols, we have the following Ricci tensors and the curvature scalar (quantities without bar and latin indices are the Finslerian quantities):

$$\begin{aligned}\bar{R}_{jk} &= \tfrac{1}{2}(R_{jk} + R_{kj}) + \tfrac{1}{2}(P_{j|k} + P_{k|j}) - P_k{}^r{}_i P_r{}^i{}_j \\ &\quad + S_{jk} - C_j{}^i{}_k|_i - C_i{}^r{}_k C_r{}^i{}_j \\ &\quad + \tfrac{1}{2}(C_j{}^a{}_r R^{\,r}{}_{ka} + C_k{}^a{}_r R^{\,r}{}_{ja}) + \tfrac{1}{4}g^{am}R_{rja}R^{\,r}{}_{kn},\end{aligned}$$

$$\bar{R}_{(j)k} = C_k|_j - C_{j|k} + \tfrac{1}{2}(g^{im}R_{jkm|i} + R^{\,r}{}_{ki}P_r{}^i{}_j + P^r R_{jrk}),$$

$$\begin{aligned}\bar{R}_{(j)(k)} &= S_{jk} - C_r{}^i{}_j C_i{}^r{}_k - C_j|_k + P_j{}^i{}_{k|i} \\ &\quad - P_r P_j{}^r{}_k + \tfrac{1}{4}g^{rm}g^{ia}R_{jim}R_{kar},\end{aligned}$$

$$\begin{aligned}\bar{R} &= R + 2S - 2C^i|_i - 2C_j{}^i{}_k C^j{}_i{}^k + 2P^i{}_{|i} - P_j{}^i{}_k P^j{}_i{}^k \\ &\quad - P^r P_r + \tfrac{3}{4}g^{jk}g^{am}R_{rkm}R^{\,r}{}_{ja},\end{aligned}$$

where

$$R \equiv g^{jk} R_{j\ ki}^{\ i},$$
$$S \equiv g^{jk} S_{j\ ki}^{\ i},$$
$$P^i \equiv g^{ir} P_r, \quad P_r \equiv P_{r\ i}^{\ i},$$
$$C^i \equiv g^{ir} C_r, \quad C_r \equiv C_{r\ i}^{\ i}.$$

The curvature scalar $\bar{R}$ reduces to the Riemannian one in the case that the metric tensor g_{ij} is a Riemannian metric, i.e., $C_{ijk} = 0$.

Now we shall construct the Einstein tensor in the tangent bundle by contracting the Bianchi second identities. Then the Einstein tensor $E^{\alpha\beta}$ in the tangent bundle is defined by

$$E^{\alpha\beta} \equiv \bar{R}_{\alpha\beta} - \tfrac{1}{2} G^{\alpha\beta} \bar{R}.$$

The Einstein tensor $E^{\alpha\beta}$ obviously satisfies the following divergenceless equations:

$$E^{\alpha\beta}{}_{;\alpha} = 0.$$

These equations are the coupled differential equations on the Finslerian curvature tensors and the Finslerian torsion tensors. The Einstein equations in a tangent bundle are now defined by

$$E^{\alpha\beta} = T^{\alpha\beta},$$

where $T^{\alpha\beta}$ is the energy–momentum tensor in the tangent bundle and should satisfy the energy–momentum conservation equation $T^{\alpha\beta}{}_{;\alpha} = 0$.

Now let us write down the vacuum Einstein equation in the tangent bundle, i.e,, $T^{\alpha\beta} = 0$. In this case $E^{\alpha\beta} = 0$ are equivalent to $\bar{R}^{\alpha\beta} = 0$. By decomposing the Ricci tensor $\bar{R}^{\alpha\beta}$ with respect to the homogeneous degrees in y, we have the following seven equations:

$$R_{jk} + R_{kj} + C_{j\ r}^{\ a} R^{\ r}_{\ ka} + C_{k\ r}^{\ a} R^{\ r}_{\ ja} + P_{j|k} + P_{k|j} - 2P_{k\ a}^{\ r} P_{r\ j}^{\ a} = 0, \tag{4.1}$$
$$g^{am} R_{jkm|a} + R^{\ r}_{\ ka} P_{r\ j}^{\ a} + R_{jrk} P^r = 0, \tag{4.2}$$
$$g^{am} R_{rja} R^{\ r}_{\ km} = 0, \tag{4.3}$$
$$g^{rm} g^{ia} R_{jim} R_{kar} = 0, \tag{4.4}$$
$$C_j|_k + C_r C_{j\ k}^{\ r} = 0, \tag{4.5}$$
$$C_{k|j} - C_{j|k} = 0, \tag{4.6}$$
$$P_{j\ k|r}^{\ r} - P_r P_{j\ k}^{\ r} = 0. \tag{4.7}$$

Multiplying (4.5) by y^j, and summing in j, also noting the fact that $y^j|_k = \delta^j_k$, we have

$$C_i = 0. \tag{4.5'}$$

Then Eq. (4.6) is automatically satisfied. By Eqs. (4.1) and (4.5') and noting the following relation derived from the Bianchi identity for $C_i = 0$,

$$R_{jk} - R_{kj} + C_{k\ r}^{\ a} R^{\ r}_{\ ja} - C_{j\ r}^{\ a} R^{\ r}_{\ ka} = 0,$$

we have

$$R_{jk} + C_{k\ r}^{\ a} R^{\ r}_{\ ja} - P_{k\ a}^{\ r} P_{r\ j}^{\ a} = 0. \tag{4.1'}$$

Conversely, if (4.1') holds, then (4.1) is satisfied. Other equations can be simplified on account of the identity $C_i = 0$. Resultant equations are

$$R_{jk} + C_{k\ r}^{\ a} R^{\ r}_{\ ja} - P_{k\ a}^{\ r} P_{r\ j}^{\ a} = 0, \tag{4.8}$$
$$g^{am} R_{jkm|a} + R^{\ r}_{\ ka} P_{r\ j}^{\ a} = 0, \tag{4.9}$$
$$g^{rm} g^{ab} R_{jbm} R_{kar} = 0, \tag{4.10}$$
$$g^{am} R_{rja} R^{\ r}_{\ km} = 0, \tag{4.11}$$
$$P^{r}_{\ jk|r} = 0, \tag{4.12}$$
$$C_i = 0. \tag{4.13}$$

To solve the set of equations (4.8), ..., (4.13) we assume that $R^{\ i}_{\ jk} = 0$ (cf. Sec. 3). Then Eqs. (4.8), ..., (4.13) can be drastically simplified.

First we notice the following relations between the Berwald's curvature tensor H_{hijk} and the Cartan's curvature tensor R_{hijk} (see Matsumoto[22]):

$$R_{hijk} = H_{hijk} + C_{hir} R^{\ r}_{\ jk} - P_{hij|k} + P_{hik|j} - Q_{hijk},$$

where

$$Q_{hijk} = P_{hrj} P_{i\ k}^{\ r} - P_{hrk} P_{i\ j}^{\ r}.$$

If $R^{\ r}_{\ jk} = 0$, then $H_{hijk} = 0$. If we consider the following identities

$$H_{hijk} - H_{ihjk} = 2(R_{hijk} + Q_{hijk}),$$
$$H_{hijk} + H_{ihjk} = 2(P_{hij|k} - P_{hik|j}) - 2C_{h\ i}^{\ r} R_{rjk},$$

we have

$$R_{hijk} = -Q_{hijk}, \tag{4.14}$$
$$P_{hij|k} - P_{hik|j} = 0. \tag{4.15}$$

From (4.15) we have

$$P_{h|k} = P_{h\ k|r}^{\ r}.$$

If further $C_i = 0$, then we get

$$P_{h\ k|r}^{\ r} = 0. \tag{4.16}$$

From (4.14) we have

$$R_{hijk} = P_{hrk} P_{i\ j}^{\ r} - P_{hrj} P_{i\ k}^{\ r},$$

and hence we obtain

$$R_{hj} = P_{h\ r}^{\ a} P_{a\ j}^{\ r} - P_{hrj} P^r.$$

If $C_i = 0$, then we have

$$R_{hj} - P_{h\ r}^{\ a} P_{a\ j}^{\ r} = 0. \tag{4.17}$$

From these formulas the independent equations in (4.8), ..., (4.13) in the case of $R^{\ r}_{\ jk} = 0$ are only (4.13).

Finally we give the example of the solution of the Eqs. (4.13) and $R^{\ i}_{\ jk} = 0$. It is known that the following Finsler metric satisfies these equations (see Sec. 2).

$$L(x, y) = \{y^1 y^2 y^3 y^4\}^{1/4}.$$

This type of Finsler metric was fully investigated by Asanov in his generalized relativity theory.[15]

In next section we shall show that this type of metric can also be obtained from the complex-manifold structure of the tangent bundle.

5. COMPLEX MANIFOLD STRUCTURE OF TANGENT BUNDLE

The complex-manifold structure of spacetime has been investigated by several authors (see, e.g., Newmann *et al.*[37]).

They used the complex structure of spacetime, however, in a rather artificial or abstract way. Penrose[37] discussed the connection between the complex-manifold structure of spacetime and the quantized theory of gravitation. In this section we try to relate tangent bundle to complex-manifold structure. This relation is based on the fact that the dimension of a tangent bundle of spacetime is precisely eight and therefore each point p of TM can be coordinatized as (x^i, y^i) or $z^i = x^i + (-1)^{\frac{1}{2}} y^i$. However this representation of $z^i(p)$ is not a covariant one and the purpose of the following discussion is to try to find the covariant way of representing a point in TM as $z^i = u^i + (-1)^{\frac{1}{2}} v^i$. If this representation is achieved we shall be able to give the realistic image of complex manifold structure.

Before doing the program we explain complex manifolds. Complex manifold M will be defined analogously to a differentiable manifolds. However, in this case a chart[38] (U_α, ϕ_α) is the following:

U_α: an open set in M,

ϕ_α: a homeomorphism from U_α to $\phi_\alpha(U_\alpha) \subset C^n$,

and the set of charts $(U_\alpha, \phi_\alpha)_{\alpha \in \mathfrak{A}}$ is an atlas if

$\phi_\alpha \phi_\beta^{-1}$ is a holomorphic function from

$\phi_\beta(U_\beta \cap U_\alpha)$ to $\phi_\alpha(U_\alpha \cap U_\beta)$.

In a complex manifold, $p \in M$ can be coordinatized by the complex numbers $(z^i(p)) \in C^n$. Let u^i and v^i be the real and imaginary parts of z^i respectively. In a complex manifold we can define a *complex structure* J by

$$J\left(\frac{\partial}{\partial u^i}\right) = \frac{\partial}{\partial v^i}, \quad J\left(\frac{\partial}{\partial v^i}\right) = -\frac{\partial}{\partial u^i},$$

or, equivalently, by

$$J\left(\frac{\partial}{\partial z^i}\right) = (-1)^{1/2} \frac{\partial}{\partial z^i},$$

where

$$\frac{\partial}{\partial z^i} = \frac{1}{2}\left(\frac{\partial}{\partial u^i} - (-1)^{1/2} \frac{\partial}{\partial v^i}\right).$$

Of course a complex manifold is a differentiable manifold with the coordinates (u^i, v^i). Then, conversely, what kind of differentiable manifold can be considered a complex manifold? It is trivial that such a manifold should have even dimension. If there exists a (1, 1)-type tensor field J In a differentiable manifold, such that $J_x^2 = -1_x$ (1_x is an identity in M_X), the manifold is said to be an *almost complex manifold* and J is called an almost complex structure on M. The almost complex manifold is actually a complex manifold if and only if J is the complex structure. The condition for a given almost complex structure J to be a complex structure, i.e., for J to be integrable, is the vanishing of the following torsion tensor N defined by

$$N(X, Y) = J[X, Y] - [JX, Y] - [X, JY] - J[JX, JY].$$

This is the famous theorem due to Newlander and Nirenberg.[39]

Now we return to our case. Following the notations in Sec. 4, we define Z_i and $\overline{Z}_i$ by

$$Z_i = \tfrac{1}{2}\{X_i - (-1)^{\frac{1}{2}} X_{(i)}\}, \quad \overline{Z}_i = \tfrac{1}{2}\{X_i + (-1)^{\frac{1}{2}} X_{(i)}\}.$$

An almost complex structure in the tangent bundle can be defined by

$$J(Z_i) = (-1)^{\frac{1}{2}} Z_i, \quad J(\overline{Z}_i) = -(-1)^{\frac{1}{2}} \overline{Z}_i.$$

The almost complex sturcture J is not, in general, a complex structure. The condition for J to be a complex structure is, by the theorem due to Newlander and Nirenberg,[39] (see also Ref. 40) $[Z_i, Z_j] = f^k_{ij} Z_k$ for some function f^k_{ij}. In our case the condition can only be fulfilled if $R^{\ i}_{jk} = 0$, i.e., the underlying Finsler space possesses an absolute parallel vector field. On physical grounds (see Sec. 3) we shall assume that the condition is fulfilled. Then there exists a complex coordinate system $\{z^i = u^i + (-1)^{\frac{1}{2}} v^i\}$ such that

$$J\left(\frac{\partial}{\partial u^i}\right) = \frac{\partial}{\partial v^i}, \quad J\left(\frac{\partial}{\partial v^i}\right) = -\frac{\partial}{\partial u^i}.$$

We can further show that the lifted metric metric in the tangent bundle can be expressed in the form (this is a consequence of the integrability condition and the fact that the connection is Cartan-type)

$$G = 2H_{l\overline{m}} dz^l d\overline{z}^m = 2\frac{\partial^2 L^2}{\partial z^l \partial \overline{z}^m} dz^l d\overline{z}^m.$$

Let $H = \det(H_{l\overline{m}})$; then the Ricci tensor can be expresses as[38]

$$K_{l\overline{m}} = -\frac{\partial^2 \ln H}{\partial z^l \partial \overline{z}^m}.$$

As a vacuum Einstein equation, we set $K_{l\overline{m}} = 0$. For the general case the relation between two coordinate systems (x^i, y^i) and (u^i, v^i) is very complicated (we have to solve a set of nonlinear differential equations) and thus here we only consider the locally-Minkowski case.[22] In this special case (x^i, y^i) itself forms a complex coordinate system, and $K_{l\overline{m}} = 0$ is equivalent to $C_{m\|l} = 0$. Hence we have $C_m = 0$ and this equation has a solution

$$L(z, \overline{z}) = \tfrac{1}{2}\left\{\prod_k (\overline{z}^k - z^k)\right\}^{1/4}.$$

(See the last paragraph in Sec. 4).

This is in contrast with the Riemannian case because the tangent bundle TM equipped with a Riemannian metric, which is the lifted metric of the "Riemannian" metric in M, can only be a complex manifold when the Riemannian metric in M is locally flat. In this respect we shall be able to construct the curved complex manifolds from a given tangent bundle which is equipped with a lifted Finsler metric.

6. CONCLUDING REMARKS

We have developed the Finslerian relativity based on the tangent bundle in previous sections. However these investigations are only concerned with the classical level. Here we shall consider the way of quantizing our theory. Recently, complex manifold technques have been under active investigation[37] and, as was discussed by Penrose, in connection with the twistor theory,[41] a complex manifold reveals quantum level theory (see also Refs. 37 and 42). To apply Penrose's methods we shall have to investigate the spinor theory in Finsler spaces in more details. Another interesting way of relating the Finsler geometry to quantum theory is "geometrical mechanics" due to Synge.[13] His methods are based on the dual relations between the Lagrangian formalism and the Hamiltonian one. Finsler geometry is well suited to the Lagrangian formalism and the Hamiltonian formalism is suited to quantum theory. Therefore we might expect that the Finsler geometry plays an important role in quantum theory. In this respect the paper of Kern[44] seems to be useful.

We end this paper by this final comment. As was quoted in Sec. 1, Drechsler's geometrical approach of gauge theory resemble the Finslerian aspect of field theory. In considering particle physics, the carrier manifold is usually assumed to be Lorentzian. To investigate the composite nature of particles such an assumption seems to be reasonable in the Finslerian aspect, the assumption corresponds to a locally-Minkowski space. Therefore it is interesting to investigate the locally-Minkowski space (e.g., $\{y^1y^2y^3y^4\}^{1/4}$) as the model that describes the composite nature of the particles (see Appendix C).

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APPENDIX A

In this appendix we shall present some of the properties of a generalized Finsler metric $g_{ij} = LL_{ij} - L_iL_j$ without proofs. In the following we shall use the same notations as those used in Sec. 2.

The torsions and the curvatures are given by:

$$R^{\,i}_{\ jk} = R_{0\ jk}^{\ i}, \tag{A1}$$

$$P_{j\ k}^{\ i} = P_{0\ jk}^{\ i} = C_{j\ k|0}^{\ i}, \tag{A2}$$

$$\begin{aligned} P_{hkji} &= P_{jki}\,|_h - P_{jhi}\,|_k + \tfrac{1}{2}(C_{jhr} + C_{hjr})P_k{}^r{}_i \\ &\quad - \tfrac{1}{2}(C_{jkr} + C_{kjr})P_j{}^r{}_i + \tfrac{1}{2}(C_{hkr} - C_{khr})P_j{}^r{}_i \\ &= C_{jik\,|h} - C_{jhi|k} + \tfrac{1}{2}(C_{jhr} + C_{hjr})P_k{}^r{}_i \\ &\quad - \tfrac{1}{2}(C_{jkr} + C_{kjr})P_h{}^r{}_i + \tfrac{1}{2}(C_{hkr} - C_{khr})P_j{}^r{}_i. \end{aligned} \tag{A3}$$

The h-curvature $R_i{}^h{}_{jk}$ and v-curvature $S_i{}^h{}_{jk}$ are given by the same forms as in Sec. 2.

By (A2) and (A3) we can easily prove the following theorem.

Theorem: The generalized Finsler metric $g_{ij} = LL_{ij} - L_iL_j$ is locally Minkowski (i.e., there exists a coordinate system such that $\partial_i g_{jk} = 0$) if and only if

$$R_{ijkl} = 0 = C_{ijk\,|0}.$$

APPENDIX B

In this appendix we shall discuss the way of obtaining one of the metrical connections of GFM. We, of course, call a symmetric nondegenerate tensor $g_{ij}(x, y)$ homogeneous of degree zero in y a generalized Finsler metric. Moór[45] discussed the connection for GFM. However he did not give the explicit form of $F_j{}^i{}_k$. Here we give one way of obtaining the metric connection for arbitrary GFM.

We shall be able to determine the v-connection parameters $C_j{}^i{}_k$ by the metrical condition $g_{ij}\,|_k = 0$. However, for the physical applications we want a Cartan-type connection so in this appendix we proceed according to the following line. First we define the function $\widetilde{L}^2(x, y) = g_{ij}(x, y)y^iy^j$ and define the reduced metric $\tilde{g}_{ij} = \widetilde{L}\widetilde{L}_{ij} + \widetilde{L}_i\widetilde{L}_j$. Corresponding to $\tilde{g}_{ij}$ we can obtain the $C\Gamma = (\widetilde{F}_j{}^i{}_k, \widetilde{N}^i{}_k, \widetilde{C}_j{}^i{}_k)$. From now on we shall determine the metrical connection for the metric g_{ij} in the form

$$F_j{}^i{}_k = \widetilde{F}_j{}^i{}_k + M_j{}^i{}_k, \quad M_j{}^i{}_k = M_k{}^i{}_j,$$

$$N^i{}_k = \widetilde{N}^i{}_k + P^i{}_k,$$

$$C_j{}^i{}_k = \widetilde{C}_j{}^i{}_k + Q_j{}^i{}_k, \quad Q_j{}^i{}_k = Q_k{}^i{}_j.$$

By the metrical condition $g_{ij}\,|_k = 0$, we can determine $C_j{}^i{}_k$ as follows:

$$C_j{}^i{}_k = \widetilde{C}_j{}^i{}_k + \tfrac{1}{2}g^{ir}[\widetilde{\nabla}_{(k)}g_{jr} + \widetilde{\nabla}_{(j)}g_{rk} - \widetilde{\nabla}_{(r)}g_{jk}],$$

where

$\widetilde{\nabla}_{(k)}$ is the v-covariant derivative with respect to $C\Gamma$.

From the condition $g_{ij|k} = 0$ we obtain

$$\begin{aligned} \widetilde{\nabla}_k g_{ij} + \widetilde{\nabla}_i g_{jk} - \widetilde{\nabla}_j g_{ki} &= 2g_{rj}M_i{}^r{}_k + P^a{}_k\partial_{(a)}g_{ij} \\ &\quad + P^a{}_i\partial_{(a)}g_{jk} - P^a{}_j\partial_{(a)}g_{ik}, \end{aligned}$$

where

$\widetilde{\nabla}_k$ is the h-covariant derivative with respect to $C\Gamma$.

To solve these equations we shall assume that $P^i{}_j = 0$. Then we can determine the h-connection parameters as follows:

$$F_j{}^i{}_k = \widetilde{F}_j{}^i{}_k + \tfrac{1}{2}g^{ir}[\widetilde{\nabla}_k g_{jr} + \widetilde{\nabla}_h g_{rk} - \widetilde{\nabla}_r g_{jk}].$$

For given nonzero $P^i{}_j$ we can also determine the h-connection parameters in a similar way.

APPENDIX C

In previous sections we obtained the fundamental function of the form $F(y) = \{y^1y^2y^3y^4\}^{1/4}$. By a transformation of a basis in the tangent space at x, we have the more general fundamental function of the form $L(x, y) = F(h_i^{\ a}(x)y^i)$. This is the special case of the 1-form type fundamental functions (see Sec. 3). In this section we shall investigate the 1-form type Finsler space, not restricted to the above type of 1-form metrics, $L(x, y) = F(h_i^{\ a}(x)y^i)\,(F(kY) = kF(Y), 0 < k)$. The metric tensor for a 1-form type fundamental function has a special form

$$g_{ij}(x, y) = h_i^{\ a}(x)h_j^{\ b}(x)H_{ab}(Y), \tag{C1}$$

where

$$Y^a = h_i^{\ a}(x)y^i$$

$$H_{ab}(Y) = \frac{1}{2}\frac{\partial^2F^2(Y)}{\partial Y^a\partial Y^b}.$$

The decomposition (C1) can be interpreted as follows. If we set up the observer's tetrad system at x by $\{h_i^{\ a}(x)\}$, then we can compensate for the (external) gravitational effects and we can observe the internal structure of the matter fields $(H_{ab}(Y))$. The four quantities (Y^a) relate the external (x) and the internal (y) degrees of freedom in the form of the scalar combinations $(h_i^{\ a}(x)y^i)$.

Let us assume that the metric tensor $H_{ab}(Y)$ has the signature -2; then we can further decompose it as follows:

$$H_{ab}(Y) = e_a^A(Y)e_b^B(Y)\eta_{AB},$$

where

$$\eta_{AB} = \mathrm{diag}(1, -1, -1, -1).$$

(This is the case for the fundamental function of the form $\{Y^1Y^2Y^3Y^4\}^{1/4}$.) Since the quantities Y^a are invariant under the coordinate transformations $x^i \rightarrow \bar{x}^i$, we may call the Y-space the internal space. As a tetrad system $\{e^A\}$ in the internal space, we can choose, without loss of generality,

$$e_a^0(Y) = Y_a/F(Y) \quad (Y_a = H_{ab}Y^b).$$

Since the physical fields are assumed to be homogeneous of degree zero in Y, we can only consider the fields on an indicatrix $I = \{Y|F(Y) = 1\}$ in Y-space. Let $u^\alpha(\alpha = 1, 2, 3)$ be the coordinates in I; then the physical quantities are the functions of (u^α). Under the transformations of the coordinates $u^\alpha \rightarrow \bar{u}^\alpha$ the internal tetrad system $\{e_a^A(Y)\}$ transforms according to

$$e^0 \rightarrow e^0$$

$$e^\alpha \rightarrow \frac{\partial \bar{u}^\alpha}{\partial u^\beta} e^\beta \equiv L_{\ \beta}^{\alpha} e^\beta.$$

Since the tetrad system $\{e^A\}$ should satisfy the relations

$$H_{ab} = e_a^A e_b^B \eta_{AB},$$

the coefficients $L_{\ \beta}^{\alpha}$ should satisfy the relations which the generators of the usual 3-rotation group should obey. In these respects, the isosymmetry can be interpreted as the coordinate transformation of the internal space, i.e., one can express the isogroup in terms of the geometrical transformations.

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Existence of localized solutions for certain model field theories [a)]

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We study the existence of static solutions of certain model equations. In particular we consider coupled systems of equations and allow the coefficients to be variable, even singular.

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1. INTRODUCTION

The study of the classical nonlinear field equations is a means of obtaining insight into the structure of the corresponding quantum field theories. Classical field theory is, at least, the zeroth order approximation to quantum field theory. Therefore a detailed understanding of the solutions of the classical equations is an essential goal.

In this paper we prove the existence, and in certain cases the nonexistence, of static solutions of certain model equations (see Secs. 3 and 4), including the well-known system of N. Rosen.[1]

The methods used are an extension of those of Ref. 2. From the mathematical point of view, the novel feature here is the replacement of $(1-\Delta)$ by $(-\Delta)$, the negative Laplacian. In addition, we consider coupled systems of equations and allow the coefficients to be variable, even singular.

2. RESULTS

By a solution $u(x)$ we will understand a function, not identically zero, which is sufficiently small at infinity (so that certain integrals converge). We consider a quadratic form

$$Q_0(u)=\tfrac{1}{2}\sum_{k,l=1}^{m} a_{kl}(r)\nabla u_k(x)\cdot\nabla u_l(x), \qquad (1)$$

where a_{kl} are certain functions of $r=|x|$ and $a_{kl}=a_{lk}$, $u=(u_1,\cdots,u_m)$, $x=(x_1,\cdots,x_n)$. $\nabla=(\partial_1,\cdots\partial_n)$. Let $K(x,u)$ be a function. We consider solutions of the variational problem

$$\delta\int[Q_0(u)+K(x,u(x))]\,dx=0 \qquad (2)$$

(integration over all space $\mathbb{R}^n$). We may write the Euler equation as

$$A_0u(x)+K'(x,u(x))=0 \text{ in } \mathbb{R}^n, \qquad (3)$$

where we denote $K'=\partial K/\partial u$ and

$$(A_0u)_k=\sum_{l=4}^{m}-\nabla\cdot[a_{kl}\nabla u_l]. \qquad (4)$$

If we multiply (3) by u and integrate, we have

$$2\int Q_0(u)\,dx+\int u(x)\cdot K'(x,u(x))\,dx=0. \qquad (5)$$

(This identity and the following ones require the integrals to be finite.) We claim that

$$2n\int K(x,u)\,dx-(n-2)\int u\cdot K'(x,u)\,dx$$
$$=-2\int\left[r\frac{\partial K}{\partial r}(x,u)-r\frac{\partial Q_0}{\partial r}(u)\right]dx. \qquad (6)$$

Identity (6) is a consequence of scale invariance. Let $u_\lambda(x)=\lambda^p u(\lambda x)$, where $p=\frac{1}{2}(n-2)$ and $\lambda>0$. Then $(\nabla u_\lambda)(x)=\lambda^{n/2}(\nabla u)(\lambda x)$ and the Lagrangian is

$$\mathscr{L}(u_\lambda)=\int[Q_0(x,\nabla u_\lambda)+K(x,u_\lambda(x))]\,dx$$
$$=\int\left[Q\left(\frac{x}{\lambda},\nabla u(x)\right)+\lambda^{-p}K\left(\frac{x}{\lambda},\lambda^{2p}u(x)\right)\right]dx.$$

Hence a solution of (2) satisfies

$$0=\frac{d}{d\lambda}\bigg|_{\lambda=1}\mathscr{L}(u_\lambda)$$
$$=\int\left[-r\frac{\partial Q_0}{\partial r}-r\frac{\partial K}{\partial r}-nK+2pu\cdot K'\right]dx.$$

Combining this result with (5) gives (6). Another derivation of (6) can be given directly from the differential equation (3), by multiplying (3) by $r\,\partial u/\partial r$ and integrating by parts. From (6) we can also express the "energy" as

$$E=\int[Q_0+K]\,dx=\frac{1}{n}\int\left[Q_0-r\frac{\partial K}{\partial r}-r\frac{\partial Q_0}{\partial r}\right]dx.$$

Now we will state the main theoretical result of this paper. For simplicity, we assume $n\geqslant 3$. We consider a quadratic form

$$Q(u)=\frac{1}{2}\sum_{k,l=1}^{m}[a_{kl}(r)\nabla u_l+b_{kl}(r)u_k\cdot u_l],$$

where $a_{kl}=a_{lk}$ and $b_{kl}=b_{lk}$ are measurable functions of $r=|x|$. We also consider two continuous functions (nonlinear terms) $G(s)$ and $H(s)$ defined for $s\in\mathbb{R}^n$. Let

$$(Au)_k=\sum_{l=1}^{m}[-\nabla(a_{kl}\nabla u_l)+b_{kl}u_l].$$

Hypotheses:

I. There is a constant $C_1>0$ such that

$$\int Q(v)\,dx\geqslant C_1\int|\nabla v|^2\,dx$$

for all C^∞ functions $v(x)$ with compact support.

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II. $G(s) \geqslant 0$, $H(0) = 0$, h is not identically zero. If $H'(s) = 0$ then $H(s) = 0$.

III. As $s \to 0$ $|H(s)| = o(|s|^{l+1} + G(s))$, where $l = 1 + 4/(n-2)$.

IV. As $|s| \to \infty$, $|H(s)| + |H'(s)| + |G'(s)| = o(|s|^{l+1} + G(s))$.

Theorem 1. There exists at least one solution of the equation

$$Au(x) + G'[u(x)] = \lambda H'[u(x)] \text{ in } \mathbb{R}^n,$$

where λ is a real number and $u(x)$ has the following properties:

$u(x)$ is not identically zero and is measurable.
$u(x)$ depends only on $r = |x|$.
$r^{1-n/2} u(x)$ is bounded, $u(0) = 0$.

$$\int \left[\frac{u^2}{r^2} + |u|^{l+1} + G(u) + |\nabla u|^2 \right] dx < \infty.$$

The theorem will be proved in Sec. 5.

3. ROSEN'S MODEL

N. Rosen *et al.*[1,3] studied a pair of coupled Maxwell and scalar fields with the Lagrangian

$$\mathscr{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} - (\partial_\mu - iA_\mu)\phi(\partial^\mu + iA^\mu)\phi^* + \phi^*\phi.$$

We have taken the mass $m = 1$ and the coupling constant $e = 1$ for simplicity. They put

$$\phi = \varphi(x) e^{-i\alpha t}, \quad A_0 = A(x), \quad A_K = 0 \ (K = 1,2,3).$$

The field equations then reduce to

$$-\Delta\varphi + \varphi = (\alpha + A)^2 \varphi,$$
$$-\Delta A = (\alpha + A)\varphi^2, \qquad (7)$$

with $A(x)$ and $\varphi(x)$ vanishing as $|x| \to \infty$, where $x \in \mathbb{R}^3$ and α is a given arbitrary constant. We shall apply Theorem 1 to show the existence of a (nontrivial) solution of (7). Let $u =$ the pair $[\varphi, A]$

$$Q(u) = \tfrac{1}{2}|\nabla\varphi|^2 + \tfrac{1}{2}|\nabla A|^2,$$
$$G(u) = \tfrac{1}{2}\varphi^2; \ H(u) = \tfrac{1}{2}(2\alpha A + A^2)\varphi^2.$$

Then $H'(u) =$ the pair $[\partial H/\partial A, \partial H/\partial\varphi] = [(\alpha + A)\varphi^2, (2\alpha A + A^2)\varphi.]$ Now we verify Hypotheses I–IV. I is obvious. If $H'(u) = 0$ then $\varphi = 0$ or $2\alpha A + A^2 = 0$, hence $H(u) = 0$. This proves II. If $u \to 0$ then $\varphi \to 0$ and $A \to 0$, hence $2\alpha A + A^2 \to 0$, hence $(2\alpha A + A^2)\varphi^2 = o(\varphi^2)$ hence $|H| = o(G)$. This proves III. As for IV it suffices to prove

$$|2\alpha A + A^2|\varphi^2 + |\alpha + A|\varphi^2 + |2\alpha A + A^2||\varphi| + |\varphi| = o(A^6 + \varphi^6)$$

as $|A| + |\varphi| \to \infty$. (Note that $l = 5$.) This is obvious since

$$2A^2\varphi^2 \leqslant A^4 + \varphi^4 = o(A^6 + \varphi^6).$$

So by Theorem 1 there exists a radial solution of the system

$$-\Delta\varphi + \varphi = \lambda(2\alpha A + A^2)\varphi \qquad (8)$$
$$-\Delta A = \lambda(\alpha + A)\varphi^2 \qquad (9)$$

for some constant λ. Multiplying (9) by $(\alpha + A)$ and integrating we have

$$\int |\nabla A|^2 dx = \lambda \int (\alpha + A)^2 \varphi^2 dx.$$

Hence $\lambda > 0$. Now we change scale to bring (8) and (9) into the form (7). Note that $2\alpha A + A^2 = (\alpha + A)^2 - \alpha^2$. We change scale $x \to (1 + \lambda\alpha^2)^{1/2} x$ to bring (8) and (9) into the form

$$-\Delta\varphi + \varphi = \mu(\alpha + A)^2\varphi,$$
$$-\Delta A = \mu(\alpha + A)\varphi^2,$$

where $\mu = \lambda(1 + \lambda\alpha^2)^{-1}$. Finally we change dependent variables $\sqrt{\mu}\varphi \to \varphi$, $\sqrt{\mu}A \to A$, and $\sqrt{\mu}\alpha \to \alpha$. This eliminates the factor μ and we obtain a solution of the system (7).

The static solution we have founded can be interpreted as a classical particle, since it concentrates charge and energy in a localized region. Rosen and Menius[3] studied this kind of radial solution numerically.

The Rosen model with a scalar self-interaction was considered by Rosen[4] and Rañada *et al.*[5] In the case of a quartic self-coupling, for instance, with $\alpha = 0$, this system is

$$-\Delta\varphi + \varphi = A^2\varphi + \beta\varphi^3,$$
$$-\Delta A = A\varphi^2, \qquad (10)$$

with $\beta > 0$.

The existence of a solution is verified as in the previous case. We have Q and G as before and

$H(u) = \tfrac{1}{2}A^2\varphi^2 + \tfrac{1}{4}\beta\varphi^4$
$H'(u) = [A\varphi^2, A^2\varphi + \beta\varphi^3]$.
II) If $H'(u) = 0$, then $A = \varphi = 0$, hence $H(u) = 0$.
III) If $A \to 0$ and $\varphi \to 0$, then $H = o(\varphi^2)$.
IV) If $A^2 + \varphi^2 \to \infty$, then $A^2\varphi^2 + \varphi^4 = o(A^6 + \varphi^6)$.

Thus there exists a non-trivial solution of the system

$$-\Delta\varphi + \varphi = \lambda(A^2\varphi + \beta\varphi^3),$$
$$-\Delta A = \lambda A\varphi^2.$$

By rescaling we find a nontrivial solution of (10).

4. FURTHER EXAMPLES

Example 1: Consider the equation

$$-\Delta u = |u|^{q-1}u, \quad q > 1,$$

where $u: \mathbb{R}^n \to \mathbb{R}^m$ is a vector field; m and n are arbitrary ($n \geqslant 3$). And under what conditions on n and q can this equation have a solution? As before, the solution should vanish at infinity, but not be identically zero. We apply identity (6) where

$$Q(u) = \tfrac{1}{2}|\nabla u|^2 \text{ and } K(u) = (q+1)^{-1}|u|^{q+1}.$$

Thus if the function

$$(n-2)u \cdot K'(u) - 2nK(u) = [n - 2 - 2n(q+1)^{-1}]|u|^{q+1}$$

is everywhere of one sign, then there is no solution. Therefore there can exist a solution *only if* $q = 1 + 4/(n-2)$. Such a solution is known[6] $u(x) = Z(Z^4/3 + |x|^2)^{-1/2}$ if $m = 1$,

$n = 3$ and Z is an arbitrary constant. When $m = 1$ and $n \geqslant 3$ it was studied by Talenti.[7]

Example 2: Consider $p \neq q$, numbers greater than one, and the equation

$$-\Delta u + |u|^{p-1}u = \lambda |u|^{q-1}u.$$

By scale changes $x \to \alpha x$ and $u \to \beta u$, we may as well assume $\lambda = \pm 1$. We take

$$K(u) = (p+1)^{-1}|u|^{p+1} - \lambda (q+1)^{-1}|u|^{q+1}.$$

If $\lambda < 0$, then $K(u) \geqslant 0$ and by (6) there is no solution. Let $\lambda = 1$. By the same reasoning as in Example 1, the function

$$[n - 2 - 2n(p+1)^{-1}]|u|^{p+1}$$
$$-[n - 2 - 2n(q+1)^{-1}]|u|^{q+1}$$

must change sign if there exists a nontrivial solution. Let $l = 1 + 4/(n-2)$. If l lies strictly between p and q, there is no solution.

Now apply Theorem 1 where $G = |u|^{p+1}/(p+1)$ and $H = |u|^{q+1}/(q+1)$. Hypotheses III and IV reduce to:

$|u|^{q+1} = o(|u|^{l+1} + |u|^{p+1})$ as $|u| \to 0$ and $|u| \to \infty$.

Therefore there exists at least one solution provided q lies strictly between l and q. (If p lies between l and q, we do not know whether there is a solution.)

Example 3: If h is a positive constant and $m \geqslant 1$, consider the equation

$$-\Delta u + hr^{-2}u - |u|^{q-1}u = 0.$$

Let $K(u) = hr^{-2}u^2/2 - |u|^{q+1}/(q+1)$ then

$$2nK - (n-2)u \cdot K'(u) + 2r\partial K/\partial r$$
$$= [n - 2 - 2n(q+1)^{-1}]|u|^{q+1}.$$

By (6) there can be a solution only if $q = 1 + 4/(n-2)$ and $n \geqslant 3$.

If there is a radial solution, the $h > h_c$ where $h_c = (n-2)(n-4)/4$. To show this, let $v = r^{-\alpha}u$, where $\alpha = 2/(q-1) = (n-2)/2$. Then

$$r(rv_r)_r + (h_c - h)v + |v|^{q-1}v = 0. \tag{11}$$

Hence

$$r^2 v_r{}^2 + (h_c - h)v^2 + 2|v|^{q+1}/(q+1) = \text{const} = 0.$$

If $h_c \geqslant h$, then each term is positive and so $v = 0$.

In fact, the conditions

$$q = 1 + 4/(n-2) \text{ and } h > h_c$$

are sufficient for the existence of a solution. If v is assumed to be a radial function, then $Lv = 0$ and

$$r(rv_r)_r - (h - h_c)v + |v|^{q-1}v = 0.$$

The final quadrature is performed easily to yield the solution

$$u(x) = Zr^{a+1-n/2}[(n-2)Z^{4/(n-2)}(4a^2n)^{-1} + r^{4a/(n-2)}]^{(n/2)-1},$$

where $a = \sqrt{h - h_c}$, $m = 1$ and Z is an arbitrary constant. This example restricted to the case $m = 1$ and $n = 3$ is in Vázquez.[8,9]

Example 4: Consider

$$-\Delta u + a(r)u - u^3 = 0,$$

where $n = 3$ and $a(r)$ is a function. This equation was studied in[10] in the case $a(r) = \text{const}$, where a solution was interpreted as a kink. It is important to understand how a kink changes in the presence of a potential, especially a Coulomb potential.

Assume that

$$a(r) \geqslant -\alpha/r^2 + \gamma, \tag{12}$$

where $\gamma > 0$ and $\alpha < \frac{1}{4}$. We will show that there exists a solution by Theorem 1. We define

$$Q(u) = \tfrac{1}{2}|\nabla u|^2 + \tfrac{1}{2}[a(r) - \gamma]u^2,$$
$$G(u) = \tfrac{1}{2}\gamma u^2,\ H(u) = \tfrac{1}{4}u^4.$$

By Lemma (at the end of Secs. 5 and 6), we have

$$2\int Q(v)\,dx \geqslant (\tfrac{1}{4} - \alpha)\int |\nabla v|^2\,dx,$$

which proves I. II is trivial. III is trivial since $u^4 = o(u^2)$ as $u \to 0$. IV is trivial since $u^4 = o(u^6)$ as $|u| \to \infty$.

An example of (12) is

$$a(r) = 1 - \epsilon r^{-1} - hr^{-2}.$$

Then (12) is satisfied if $-\infty < h < \frac{1}{4}$ and $-\infty < \epsilon < \epsilon_h$, where ϵ_h is a certain positive number depending oh h. The Coulomb potential here has charge Ze where $e \sim (137)^{-1/2}$ and $h = Z^2e^4$. Our condition for existence of a solution ($h < 1/4$) means that $Z < 137/2$.

Example 5: This is a coupled system where one of the fields is very powerful at the origin. It is

$$-\Delta u + u = (1+u)^2 v,$$
$$-\Delta v + \nabla(r^{-1}\Delta v) = (1+u)v^2,$$

for $x \in \mathbb{R}^3$. The quadratic from $Q(u,v) = \frac{1}{2}|\nabla u|^2 + \frac{1}{2}(1 + r^{-1})|\nabla v|^2$ satisfies Hypothesis I. So our discussion in Sec. 3 proves the existence of a radial solution.

Proof of theorem 1: We define the inner product

$$(u,v) = \int \sum [\tfrac{1}{2}a_{kl}\nabla u_k \cdot \nabla V_l + b_{kl}u_k v_l]\,dx$$

and the norm

$$\|u\| = (u,u)^{1/2} = \left(\int Q(u)dx\right)^{1/2}.$$

A function on $\mathbb{R}^n$ is called radial if it depends only on $r = |x|$. Let X be the completion with respect to the norm $\|\|$ of the set of radial C^∞ functions with compact support. Because of Hypothesis I, the only element of X with norm zero is the zero function. Thus X is a Hilbert space. By Sobolev's inequality,

$$\left(\int |u|^{l+1}dx\right)^{1/l+1} \leqslant C\left(\int |\nabla u|^2 dx\right)^{1/2}.$$

Hence,

$$X \subset \{u \in L^{l+1} \mid u \text{ is radial and } \nabla u \in L^2\}.$$

Lemma 1: There is a constant C such that

$$|u(r)| \leqslant Cr^{1-n/2}\left(\int |\nabla u|^2 dx\right)^{1/2},$$

for all $u \in X$ and $n \geqslant 3$.

Proof: We may assume that $u \in C^\infty$ has compact support. Then

$$u(r) = -\int_r^\infty u'(\rho)\rho^{(n-1)/2}\cdot\rho^{(1-n)/2}\, d\rho.$$

By Schwarz's inequality, this is less than

$$C\left(\int |u'|^2 dx\right)^{1/2} r^{1-n/2}. \qquad \text{Q.E.D.}$$

Lemma 2: Let $N > 0$. Let ζ_N be a C^1 function of $|s|$, $s \in \mathbb{R}^m$ such that

$$\zeta_N(s) = \begin{cases} s & |s| \leqslant N \\ 2N & |s| \geqslant 2N \end{cases}$$

and $0 \leqslant \zeta'_N(s) \leqslant 1$. Define

$$G_N(s) = G(\zeta_N(s)), \quad H_N(s) = H(\zeta_N(s)).$$

Then III and IV are valid for G_N and H_N uniformly in N.

Proof: III is trivial since $G_N = \epsilon$ and $H_N = H$ for $|s| \leqslant N$. Now consider IV, it is trivial if $N \geqslant |s|$. Let $\epsilon > 0$. Let s_0 be so large that

$$|H(s)| + |H'(s)| + |G'(s)| < \epsilon(|s|^{l+1} + G(s))$$

for $s \geqslant s_0$. If $s_0/2 \leqslant N \leqslant |s|/2$ then

$$\begin{aligned} &|H_N(s)| + |H'_N(s)| + |G'_N(s)| \\ &\quad = |H(2N)| \leqslant \epsilon(|2N|^{l+1} + G(2N)) \\ &\quad \leqslant \epsilon(|s|^{l+1} + G_N(s)). \end{aligned}$$

If $|s|/2 < N < |s|$ then

$$\begin{aligned} &|H_N(s)| + |H'_N(s)| + |G'_N(s)| \\ &\quad \leqslant |H(\zeta_N(s))| + |H'(\zeta_N(s))| + |G'(\zeta_N(s)| \\ &\quad \leqslant \epsilon(|\zeta_N(s)|^{l+1} + G(\zeta_N(s))) \leqslant \epsilon(|s|^{l+1} + G_N(s)). \end{aligned}$$

Thus IV is valid for G_N and H_N uniformly for $N \geqslant s_0/2$.

Lemma 3: Given $N > 0$, there exists a nontrivial solution u_N of the problem

$$\begin{aligned} &\min \mathscr{L}_N(u) \\ &\quad = \min \int [Q(u) + (1/N)|u(x)|^2 + G_N(u(x))]\, dx \end{aligned}$$

subject to the constraints

$$u \in X \text{ and } \int H_N(u(x))\, dx = \text{const}.$$

It satisfies the variational equation

$$Au_N + (1/N)u_N + G'_N(u_N) = \lambda_N H'_N(u_N) \qquad (13)$$

for some Lagrange multiplier λ_N, where

$$(Au)_k = \sum_l [-\nabla(a_{kl}\nabla u_l) + b_{kl}u_l].$$

Proof: Since G_N is a bounded function $\mathscr{L}_N$ is a C^1 functional on X. Since H_N is bounded, the constraint is also of C^1 functional on X. Therefore any solution of the minimum problem must satisfy the variational equation (13). Now $H_N \geqslant 0$. For a large enough N, H_N is not identically zero. Therefore there exists a radial C^∞ function $U_0(x)$ of compact support such that

$$\int H(U_0(x))\, dx = \gamma > 0.$$

We assume that $N \geqslant N_0 > \max|u_0(x)|$. Let L be the minimum we are trying to achieve. Choose any minimizing sequence $u_0 \in X$ such that

$$\mathscr{L}_N(u_\nu) \searrow L, \qquad \int H_N(u_\nu)\, dx = \gamma.$$

Because of the positivity of Q and G_N, $\{u_\nu\}$ is bounded in X and $\int G_N(u_\nu)\, dx$ is bounded. By the Rellich compactness theorem, there is a subsequence (still denoted by $\{u_\nu\}$) converging to a limit u almost everywhere and weakly in X, hence in the sense of distributions. Hence $G_N(u_\nu) \to G(u)$ and $H_N(u_\nu) \to H(u)$ a.e. By Lemma 1, $u_\nu(x) \to 0$ as $|x| \to \infty$ uniformly in ν. We now apply the compactness lemma of Ref. 7. This is where III and IV come in. We conclude that

$$\int H_N(u_\nu)\, dx \to \int H_N(u)\, dx \text{ as } \nu \to \infty.$$

Hence $\int H_N(u)\, dx = \gamma$. By Fatou's Lemma and the weak convergence

$$\mathscr{L}_N(u) \leqslant \liminf \mathscr{L}_N(u_\nu) \leqslant L.$$

Hence $\mathscr{L}_N(u) = L$ and u attains the minimum.

We now complete the proof of Theorem 1. Let $u_0(x)$ be chosen as above. Let $N \geqslant N_0$. Let u_N denote the solution of Lemma 3. Then

$$\begin{aligned} \mathscr{L}_N(u_N) \leqslant \mathscr{L}_N(u_0) &= \int \left[Q(u_0) + \frac{1}{N}|u_0|^2 + G_N(u_0)\right] dx \\ &\leqslant \int \left[Q(u_0) + \frac{1}{N_0}|u_0|^2 + G(u_0)\right] dx. \end{aligned}$$

Hence $\|u_N\|$, $N^{-1}\int |u_N|^2\, dx$, and $\int G_N(u_N)\, dx$ are all bounded (independently of N). Now let v be any C^∞ function with compact support. We multiply equation (13) by v and integrate to obtain

$$\begin{aligned} &(u_N, v) + \frac{1}{N}\int u_N v\, dx + \int G'_N(u_N) v\, dx \\ &\quad = \lambda_N \int H'_N(u_N) v\, dx. \end{aligned} \qquad (14)$$

Each term on the left side of (14) is bounded, using IV. Hence the right side is also bounded.

From these bounds we deduce the convergence of a subsequence (still denoted by $\{u_N\}$) such that:

$u_N \to u$ weakly in X and a.e.

Hence $G_N(u_N) \to G(u)$, $H_N(u_N) \to H(u)$, $G'_N(u_N) \to G'(u)$ and $H'_N(u_N) \to H'(u)$ almost everywhere. Applying the Compactness lemma of Ref. 7 again, we deduce that

$$G'_N(u_N) \to G(u) \text{ and } H'_N(u_N) \to H(u)$$

locally in L^1 and that

$$\int |H_N(u_N) - H(u)|\, dx \to 0.$$

Hence $\int H(u)\, dx = \gamma$ and so u is not identically zero.

We claim that λ_N is bounded. If not, there would be a subsequence of λ_N tending to infinity. By (14) we would have

$$\int H'_N(u_N)v\,dx \to 0.$$

Hence $\int H'(u)v\,dx \to 0$. Since v is arbitrary, $H'(u) = 0$. Hence $H(u) \equiv 0$. This contradicts the fact that $\int H(u)\,dx \neq 0$.

So we may assume that $\lambda_N \to \lambda$, where λ is finite. Now each term in (13) converges as $N \to \infty$. In the limit we obtain

$$(u,v) + \int G'(u)v\,dx = \lambda \int H'(u)v\,dx,$$

for all such v. Finally, Fatou's Lemma implies that $\int G(u)dx$ is finite. It remains to show that u^2/r^2 is integrable. This follows immediately from the:

Lemma: For each $v \in X$

$$\int v^2 |x|^{-2}\,dx \leqslant 4(n-2)^{-2} \int |\nabla v|^2\,dx.$$

Proof: It suffices to prove it for C^∞ functions with compact support. In fact we will not need to assume v is radial. An elementary calculation shows

$$\nabla\cdot(xv^2/r^2)$$
$$= x\cdot 2v\nabla v/r^2 + v^2\nabla\cdot(x/r^2) = 2vv_r/r + (n-2)v^2/r^2.$$

Integrate this identity over $\mathbb{R}^n$ to get

$$(n-2)\int (v^2/r^2)\,dx$$
$$= -2\int (v/r)v_r\,dx \leqslant 2\Big(\int v^2/r^2\,dx\Big)^{1/2}\Big(\int v_r^{\,2}\,dx\Big)^{1/2}.$$

Divide by the first square root and the inequality follows. Q.E.D.

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Quantum mechanics and stochastic control theory

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A time-symmetric stochastic control theory is proposed as one of the representatives of quantum mechanics. The main idea is based on Nelson's probability theoretical approach to quantum mechanics. His approach is reformulated as a time-symmetric stochastic control problem. Several different control constraints equivalent to Nelson's are obtained. One of them has a close connection to the Lagrangian formalism of classical mechanics. This suggests to us the use of stochastic calculus of variations. Within the realm of this time-symmetric stochastic control theory it is shown why Schrödinger's original variational method of quantization was successful. Several advantageous points of the stochastic control theoretical approach to quantum mechanics, including the analysis of the classical limit, are also discussed.

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1. INTRODUCTION

Quantum mechanics has been cast into several different forms in such a way that each of them has a close correspondence to one of the different formulations of classical mechanics. For instance, starting from the Hamiltonian formalism, Heisenberg obtained the matrix mechanics (HMM). A short time later, Schrödinger obtained the wave mechanics (SWM), starting from the Hamilton–Jacobi formalism. We had to wait two decades for the appearance of the notion of Lagrangian in the literature of quantum mechanics. It was Feynman who proposed the path integral description of quantum mechanics (FPI) starting from the Lagrangian formalism.[1]

Nowadays it is widely believed that quantum mechanics has a conceptual structure of complementarity as illustrated in the following symbolic equation:

$$\text{(quantum mechanics)} = \text{(HMM)} \cup \text{(SWM)} \cup \text{(FPI)} \cup \text{(something else)}. \quad (1.1)$$

Here one can not replace the symbol "union" $\cup$ by the symbol "sum" $\oplus$ because intersections of them are not empty.

In the present paper I want to suggest another conceptual complementarity structure of quantum mechanics not illustrated by Eq. (1.1), but by a new symbolic equation

$$\text{(quantum mechanics)} = \text{(HMM)} \cup \text{(SWM)} \cup \text{(FPI)} \cup \text{(NSM)} \cup \text{(something else)}, \quad (1.2)$$

where NSM denotes Nelson's stochastic mechanics,[2–5] thought I do not concern myself with the conceptual status of NSM itself. Simply, I want to suggest the validity of Eq. (1.2) and civilize NSM in the realm of quantum mechanics in pedagogical way, that is, by showing the natural correspondence between Eq. (1.2) and the well-known conceptual complementarity structure of classical mechanics:

$$\text{(classical mechanics)} = \text{(Hamilton)} \cup \text{(Hamilton–Jacobi)} \cup \text{(Lagrange)} \cup \text{(Newton)} \cup \text{(something else like Liouville)}. \quad (1.3)$$

To do so, it seems necessary to investigate NSM in a profound way. I think that Eq. (1.2) should be believed only after clarifying the basic characters and the specific features of NSM which can not be achieved by the other representatives of quantum mechanics and also pointing out the interesting mathematical structure involved in NSM. Hence I organize the present paper as follows.

In Sec. 2 I show that the mathematical structure involved in NSM is that of the stochastic control theory. Sec. 3 is devoted to developing the time-symmetric stochastic control theoretical formulation of quantum mechanics based on NSM. Schrödinger's variational method of quantization in SWM is revisited within the realm of the stochastic control theory in Sec. 4. Several topics of quantum mechanics are chosen and investigated in the light of NSM for the purpose of clarifying the basic characters and the specific features of NSM in the same section. Discussions on the classical limit of quantum mechanics is given in Sec. 5. The last section (Sec. 6) is reserved for short concluding remarks. The theory of stochastic calculus of variations is presented in the Appendix in a compact form.

2. A MATHEMATICAL STRUCTURE INVOLVED IN NSM

This section is devoted to an exposition of NSM with an emphasis on its time-symmetric stochastic control theoretical character.

Let $[I,F] \subset \mathbb{R}$ be a finite time interval and $\mathbb{R}^n$ be an n-dimensional configuration space. A random process in $\mathbb{R}^n$ is given when a probability measure Prob is defined on a σ-algebra $\mathscr{D}$(Prob) of measurable subsets of the sample (path) space $\Omega = \Pi_{I \leqslant t \leqslant F} \mathbb{R}^n$. Position of the random process at time t is a random variable defined by

$$x(t,\omega) = \omega_t, \quad (2.1)$$

where ω_t is a cross section of a sample path $\omega \in \Omega$ at time t.

I shall consider the quantization problem of a Newtonian conservative system in classical mechanics in the language of the probability space $(\Omega, \mathscr{D}(\text{Prob}), \text{Prob})$. The Newtonian conservative system is a dynamical system of class C^2, $x(\cdot)$: $[I,F] \to \mathbb{R}^n$, described by Newton's equation of motion,

$$m\ddot{x}(t) = -\operatorname{grad} V(x(t)), \quad (2.2)$$

with initial conditions $x(I) = x_I$ and $\dot{x}(I) = v_I$, where m is a mass paramter and $V(\cdot)$: $\mathbb{R}^n \to \mathbb{R}$, class C^1, is the potential energy of the system.[6,7] It was Nelson who investigated such a quantization problem systematically.[2-5] His formalism is frequently called NSM. Let us explain NSM in terms of the stochastic control theory.

The Newtonian conservative system (2.2) is reformulated as a solution to an ordinary (differentiable) control problem

$$\dot{x}(t) = v(x(t),t;V), \tag{2.3}$$

where the control variable $v(\cdot,t;V)$ is controlled to satisfy the control constraint (2.2) for each time $t \in [I,F]$ and the initial constrtraints $x(I) = x_I$ and $v(x_I,I;V) = v_0$.[8] Here the potential energy V plays a role of control parameter. Correspondingly, quantum mechanics of the Newtonian system (2.2) is obtained as a solution to a time-symmetric stochastic control problem

$$dx(t,\omega) = b(x(t,\omega),t;V)dt + (\hbar/2m)^{1/2}dw(t,\omega), \tag{2.4}$$

where the control variable $b(\cdot,\cdot;V)$: $\mathbb{R}^n \times [I,F] \to \mathbb{R}^n$ is controlled to satisfy a control constraint

$$m\tfrac{1}{2}(DD_* + D_*D)x(t,\omega) = -\operatorname{grad} V(x(t,\omega)), \tag{2.5}$$

for each time $t \in [I,F]$ with probability one and initial constraints

$$\operatorname{Prob}(\{x(I,\omega) \in d^n x\}) = p_I(x)d^n x \tag{2.6}$$

and

$$b(\cdot,I;V) = b_I(\cdot) \tag{2.7}$$

for given $p_I(\cdot) \in L_1(\mathbb{R}^n)$ and $b_I(\cdot)$: $\mathbb{R}^n \to \mathbb{R}^n$ of class C^2. The random process $x(t,\omega)$, $I \leqslant t \leqslant F$, solving the above time-symmetric stochastic control problem, illustrates the quantum mechanical time evolution of the Newtonian conservative system (2.2)

Now I explain the notions and the notations used here. Equation (2.4) is a stochastic differential equation of Itô type and $w(t,\omega)$, $I \leqslant t \leqslant F$, is a Wiener process in $\mathbb{R}^n$ with a unit diffusion constant.[9,10] Planck's constant appears in this equation. For each fixed control variable $b(\cdot,\cdot;V)$, Eq. (2.4) generates a Markov process in $\mathbb{R}^n$.[10] D and D_* are Nelson's mean forward and backward derivatives defined by

$$Df(x(t,\omega),t) = \lim_{h \downarrow 0} h^{-1}\mathbb{E}[f(x(t+h,\omega),t+h) - f(x(t,\omega),t) | \mathscr{P}_t], \tag{2.8}$$

and

$$D_* f(x(t,\omega),t) = \lim_{h \downarrow 0} h^{-1}\mathbb{E}[f(x(t,\omega),t) - f(x(t-h,\omega),t-h) | \mathscr{F}_t], \tag{2.9}$$

respectively, for any function of position and time of class C^2.[3] Here $\mathscr{P}_t$ and $\mathscr{F}_t$ are σ-algebras generated by $[x(s,\omega) | I \leqslant s \leqslant t]$ and $[x(s,\omega) | t \leqslant s \leqslant F]$, respectively, and $\mathbb{E}[\cdot | \mathscr{A}]$ denotes the conditional expectation with respect to a σ-algebra $\mathscr{A} \subset \mathscr{D}$(Prob). These mean forward and backward derivatives are natural extensions of the ordinary time derivative. It is a well-known fact that a Markov process generated by a stochastic differential equation of Itô type is not differentiable in the usual sense. Therefore Eq. (2.5) should be understood as a natural extension of Newton's equation of motion (2.2). From the stochastic control theoretical point of view, it is convenient to relate the mean backward derivative D_* with a mean "forward" derivative of the time-reversed process. Let $\omega \in \Omega$ be a sample path of the random process $x(t,\omega)$, $I \leqslant t \leqslant F$, in question. Then the position of the time-reversed process at time $s = F - t \in [I,F]$ is defined by

$$x_*(s,\omega) = \omega_{F-s} = \omega_t = x(t,\omega). \tag{2.10}$$

By definition we have

$$D_* x(t,\omega) = -Dx_*(s,\omega). \tag{2.11}$$

Nagasawa's general theory of time reversals of Markov processes[11] claims that $x_*(s,\omega)$, $I \leqslant s \leqslant F$, is a Markov process generated by a stochastic differential equation of Itô type

$$dx_*(s,\omega) = b_*'(x_*(s,\omega),s;V)ds + (\hbar/2m)^{1/2}dw_*(s,\omega), \tag{2.12}$$

where $w_*(s,\omega)$, $I \leqslant s \leqslant F$, is a time-reversed Wiener process and $b_*'(\cdot,s;V)$ is related with $b(\cdot,t;V)$ through a relation

$$-b_*'(\cdot,s;V) = b(\cdot,t;V) - (\hbar/2m)\operatorname{grad}\log p(\cdot,t;V), \tag{2.13}$$

where $p(\cdot,t;V) \in L_1(\mathbb{R}^n)$ is a probability distribution density of $x(t,\omega)$, that is, $\operatorname{Prob}(\{x(t,\omega) \in d^n x\}) = p(x,t;V)d^n x$. By Eqs. (2.11), (2.12), and (2.13), we obtain

$$D_* x(t,\omega) = b_*(x(t,\omega),t;V) = b(x(t,\omega),t;V) - (\hbar/2m)\operatorname{grad}\log p(x(t,\omega),t;V). \tag{2.14}$$

Nelson's mean velocity $\tfrac{1}{2}(D + D_*)x(t,\omega)$ is a natural extension of the usual notion of velocity.[3]

Equivalence of the time-symmetric stochastic control problem, (2.4), (2.5), (2.6), and (2.7), to one of the other representatives of quantum mechanics, that is, SWM, was shown by Nelson with an additional integrability constraint

$$\tfrac{1}{2}(D + D_*)x(t,\omega) = (\hbar/m)\operatorname{grad}S(x(t,\omega),t;V), \tag{2.15}$$

for each time $t \in [I,F]$ with probability one and an integrable initial constraint

$$b_I(\cdot) = (\hbar/m)\operatorname{grad}B_I(\cdot), \tag{2.16}$$

for certain scalars $S(\cdot,t;V)$ and $B_I(\cdot)$ of class C^2. Namely, replacing the stochastic differential equation (2.4) by the equivalent Fokker–Planck equation

$$\frac{\partial}{\partial t}p(x,t;V) = -\operatorname{div}[b(x,t;V)p(x,t;V)] + (\hbar/2m)\operatorname{div}\operatorname{grad}p(x,t;V), \tag{2.17}$$

he found that the time-symmetric stochastic control problem in question is equivalent to a Cauchy problem for the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi(x,t;V) = -(\hbar^2/2m)\operatorname{div}\operatorname{grad}\psi(x,t;V) + V(x)\psi(x,t;V), \tag{2.18}$$

with an initial condition

$$\psi(\cdot,I;V) = \psi_I(\cdot) = p_I(\cdot)^{1/2}\exp[iS_I(\cdot)], \tag{2.19}$$

where $S_I(\cdot) = B_I(\cdot) - \frac{1}{2}\log p_I(\cdot)$. In other words, a solution to the time-symmetric stochastic control problem (2.4), (2.5), (2.6), and (2.7) with the integrability constraints (2.15) and (2.16), call it an integrable solution, can be constructed as follows. Firstly, solve the Cauchy problem (2.18) and (2.19) for the given control parameter V, i.e., the potential energy. Secondly, perform a polar decomposition of the solution $\psi_o(\cdot,t;V) \in L_2(\mathbb{R}^n)$, $I \leqslant t \leqslant F$ in the form

$$\psi_o(\cdot,t;V) = p_o(\cdot,t;V)^{1/2}\exp[iS_o(\cdot,t;V)]. \tag{2.20}$$

Thirdly, calculate an integrable vector

$$b_o(\cdot,t;V) = (\hbar/m)\,\mathrm{grad}S_o(\cdot,t;V) + (\hbar/2m)\,\mathrm{grad}\,\log p_o(\cdot,t;V). \tag{2.21}$$

Then this vector field is nothing but an integrable solution to the time-symmetric stochastic control problem in question.

It seems worthwhile to notice here that NSM has an interesting mathematical structure closely related with the time-symmetric stochastic control theory rather than with the usual theory of random processes. This is the very crucial point in understanding NSM, though it has not been recognized for a long time. The only exception is Blaquiere's paper[2] in which a stochastic control theoretical formulation of SWM is proposed independent of NSM.[13,14] Really it was independent of NSM, it appeared just before Nelson's paper.[2]

Now I want to emphasize the validity of Eq. (1.2) as we know that the present time-symmetric stochastic control problem with the integrability constraint is equivalent to SWM and gives us an interesting mathematical structure as a representative of quantum mechanics. NSM, in its present stochastic control theoretical form, provides us with a new viewpoint in understanding quantum mechanics because it has some basic characters and specific features which can not be achieved by the other representatives of quantum mechanics. This will be clarified in the following sections.

3. STOCHASTIC CONTROL PROBLEMS AS QUANTUM MECHANICS

As we have seen in the preceding section, the intersection of NSM and SWM is not empty, that is, (NSM) = (SWM) if restricted to Newtonian conservative systems and integrable solutions. Therefore it seems not so meaningless to consider the totality of stochastic control problems equivalent to (2.4) and (2.5) as a representative of quantum mechanics different from the others. By the notion of NSM, I also denote the totality of such stochastic control problems. It may or may not be more general than the others, depending on the character of each dynamical system considered.

In this section, I show the existence of time-symmetric stochastic control problems equivalent to the original one appearing in the preceding section. This will help us to make the mathematical structure of NSM more refined and fruitful.

Let us consider the Newtonian conservative system (2.2) and the equivalent ordinary control problem (2.3) and (2.2). From the point of view of classical mechanics, the control constraint (2.2) can be replaced by the energy conservation constraint

$$(m/2)|\dot{x}(t)|^2 + V(x(t)) = E, \tag{3.1}$$

for each time $t \in [I,F]$, where E is a conserved energy of the system. Correspondingly, in NSM. I have the following.

Theorem 1. The time-symmetric stochastic control problem (2.4), (2.5), (2.6), and (2.7), with the integrability constraints (2.15) and (2.16), allows us to replace the control constraint (2.5), that is, Newton's equation of motion in a generalized sense, by the energy conservation constraint in a generalized sense,

$$\mathbb{E}[\tfrac{1}{2}\{[m/2)|Dx(t,\omega)|^2 + (m/2)|D_* x(t,\omega)|^2\} + V(x(t,\omega))] = E, \tag{3.2}$$

for each time $t \in [I,F]$.

Proof of this theorem was also given by Nelson.[5]

By Eq. (3.2) one finds the notion of kinetic energy of the random process $x(t,\omega)$, $I \leqslant t \leqslant F$,

$$\mathrm{KE} = \tfrac{1}{2}[(m/2)|Dx(t,\omega)|^2 + (m/2)|D_* x(t,\omega)|^2]. \tag{3.3}$$

This is a natural extension of the classical notion of kinetic energy.

Furthermore, in NSM, quantum mechanical stationary states are characterized as solutions to the time-symmetric stochastic control problem (2.4), (2.5), (2.6), and (2.7) which satisfy an additional control constraint

$$Dx(t,\omega) = -D_* x(t,\omega), \tag{3.4}$$

for each time $t \in [I,F]$.[3] By virtue of Eq. (2.11), this constraint controls the solutions to be symmetric in probability law with respect to the time inversion. In other words, each quantum mechanical stationary state is an optimally controlled solution to the time-symmetric stochastic control problem in question in which there are no prefered directions of time. Then I have the following.

Theorem 2. The time-symmetric stochastic control problem (2.4) and (2.5) with the control constraint (3.4) reduces to the following for $I = 0$ and $F = \infty$:

$$dx(t,\omega) = b\,(x(t,\omega);V)dt + (\hbar/2m)^{1/2}dw(t,\omega). \tag{3.5}$$

Here the control variable $b\,(\cdot;V)$ is controlled to satisfy a control constraint

$$\mathbb{E}\left[\lim_{T\to\infty}\sup T^{-1}\int_0^T [(m/2)|Dx(t,\omega)|^2 + V(x(t,\omega)) - E\,]dt\right] = \text{extremal} \tag{3.6}$$

Proof: Suppose $b_o(\cdot,t;V)$ solves Eqs. (2.4) and (2.5). (Subscript o means "optimal.") By Eq. (2.14) and the Fokker–Planck equation (2.17), $b_o(\cdot,t;V)$ becomes constant in time. So I put $b_o(\cdot;V) = b_o(\cdot,t;V)$. The control constraints (2.4) and (3.4) demand

$$Dx(t,\omega) = -D_* x(t,\omega) = b_o\,(x(t,\omega);V), \tag{3.7}$$

and Eq. (2.5) becomes

$$-(m/2)\,\mathrm{grad}|b_o\,[x(t,\omega);V\,]|^2 - (\hbar/2)\,\mathrm{div}\,\mathrm{grad}b_o(x(t,\omega);V) = -\mathrm{grad}V(x(t,\omega)). \tag{3.8}$$

As $b_o(\cdot;V)$ satisfies the integrability constraints (2.15) and (2.16), Eq. (3.8) yields

$$(m/2)|b_o(x(t,\omega);V)|^2 + (\hbar/2)\,\mathrm{div} b_o(x(t,\omega);V) = V(x(t,\omega)) - E, \quad (3.9)$$

where E is a constant of integration. This can be written in a form

$$-(\hbar/2)\,\mathrm{div} b_o(x(t,\omega);V) + \underset{b}{\mathrm{ext}}[(m/2)|b(x(t,\omega);V)|^2 - mb(x(t,\omega);V)\cdot b_o(x(t,\omega);V) + V(x(t,\omega)) - E] = 0, \quad (3.10)$$

where $\mathrm{ext}_b[\cdot]$ means to take an extremal value over all possible control variables $b(\cdot;V)$ of class C^2. Let $B_o(\cdot;V)$ be a scalar such that,

$$b_o(\cdot;V) = (\hbar/m)\,\mathrm{grad} B_o(\cdot;V), \quad (3.11)$$

then Eq. (3.11) becomes

$$\underset{b}{\mathrm{ext}}[-\hbar[b\cdot\mathrm{grad} + (\hbar/2m)\,\mathrm{div\,grad}]B_o(x(t,\omega);V) + (m/2)|b(x(t,\omega);V)|^2 + V(x(t,\omega)) - E] \quad (3.12)$$

Existence of $B_o(\cdot;V)$ comes from the integrability of $b_o(\cdot;V)$. Integrating both sides of Eq. (3.12) over an interval $[0,T]$, $T>0$, dividing by T, and using the chain rule in stochastic calculus,[10] I obtain,

$$-\hbar[B_o(x(T,\omega);V) - B_o(x(0,\omega);V)]/T + \text{martingale} + \underset{b}{\mathrm{ext}}\left[T^{-1}\int_0^T[(m/2)|b(x(t,\omega);V)|^2 + V(x(t,\omega)) - E]dt\right] = 0. \quad (3.13)$$

Now what is left for us is to take the expectation and to pass to the limit $T\to\infty$, obtaining

$$\underset{b}{\exp}\left[\mathbb{E}\left[\limsup_{T\to\infty} T^{-1}\int_0^T\{(m/2)|Dx(t,\omega)|^2 + V(x(t,\omega)) - E\}dt\right]\right] = 0. \quad (3.14)$$

This claims that the time-symmetric stochastic control problem (2.4), (2.5), and (3.4) is equivalent to (3.5) and (3.6). QED

In the case of quantum mechanical ground states, Theorem 2 reduces to that of Holland.

Because Eq. (3.14) can be interpreted

$$\underset{b}{\mathrm{ext}}\left[\mathbb{E}\left[\limsup_{T\to\infty} T^{-1}\int_0^T(\mathrm{KE}+\mathrm{PE})dt\right]\right] = E, \quad (3.15)$$

where PE denotes the potential energy $V(x(t,\omega))$, I can conclude that the quantum mechanical stationary states are represented by control variables $b_o(\cdot;V)$ (i.e., optimal solutions) which extremize the mean energy of the system

$$\mathbb{E}\left[\limsup_{T\to\infty} T^{-1}\int_0^T(\mathrm{KE}+\mathrm{PE})dt\right]. \quad (3.16)$$

Discrete values of energy of the quantum mechanical stationary states appear as extremal values of the mean energy of the system (3.16) in NSM.

Next, I shall consider a Newtonian system, $x(\cdot):[I,F]\to\mathbb{R}^n$, in classical mechanics with a charge degree of freedom,

$$m\ddot{x}(t) = -e\left[\mathrm{grad}\Phi(x(t),t) + \frac{\partial}{\partial t}A(x(t),t)\right] + e[\mathrm{grad}\wedge A(x(t),t)]\cdot\dot{x}(t), \quad (3.17)$$

Here $\Phi(\cdot,\cdot)$ and $A(\cdot,\cdot)$ are time-dependent scalar and vector electromagnetic potentials, and e is a charge parameter and $\wedge$ denotes the antisymmetric tensor product. Smoothness of the electromagnetic potentials are assumed. In NSM, quantum mechanics of the Newtonian system (3.17) can be obtained as a solution to a time-symmetric stochastic control problem

$$dx(t,\omega) = b(x(t,\omega),t;\Phi,A)dt + (\hbar/2m)^{1/2}dw(t,\omega), \quad (3.18)$$

where the control variable $b(\cdot,t;\Phi,A)$ is controlled to satisfy a control constraint,

$$m\tfrac{1}{2}(DD_* + D_*D)x(t,\omega) = -e\left[\mathrm{grad}\Phi(x(t,\omega),t) + \frac{\partial}{\partial t}A(x(t,\omega),t)\right] + e[\mathrm{grad}\wedge A(x(t,\omega),t)]\cdot\tfrac{1}{2}(D+D_*)x(t,\omega), \quad (3.19)$$

for each time $t\in[I,F]$ with probability one, and the initial constraints (2.6) and (2.7). Indeed, Nelson[3] showed that with an additional integrability constraint,

$$m\tfrac{1}{2}(D+D_*)x(t,\omega) + eA(x(t,\omega),t) = \hbar\,\mathrm{grad}S(x(t,\omega),t;\Phi,A), \quad (3.20)$$

for each time $t\in[I,F]$ with probability one, the time-symmetric stochastic control problem (3.18), (3.19), (2.6), and (2.7) is equivalent to a Cauchy problem

$$i\hbar\frac{\partial}{\partial t}\psi = [(1/2m)|-i\hbar\,\mathrm{grad} - eA|^2 + e\Phi]\psi, \quad (3.21)$$

for the wavefunction $\psi(\cdot,t;\Phi,A) = p(\cdot,t;\Phi,A)^{1/2}\times\exp[iS(\cdot,t;\Phi,A)]\in L_2(\mathbb{R}^n)$, where $p(\cdot,t;\Phi,A)\in L_1(\mathbb{R}^n)$ denotes the probability distribution density of $x(t,\omega)$. Of course, the initial condition for the Cauchy problem (3.21) must be chosen in a way consistent with the initial constraints (2.6) and (2.7) and the integrability constraint (3.20).

In classical mechanics, the Newtonian system (3.17) is reformulated as a Lagrangian ordinary control problem

$$\dot{x}(t) = v(x(t),t;\Phi,A), \quad I\leqslant t\leqslant F, \quad (3.22)$$

where the control variable $v(\cdot,\cdot;\Phi,A)$ is controlled to satisfy a variational constraint

$$\delta\int_I^F L(x(t),\dot{x}(t);\Phi,A)dt = 0, \quad (3.23)$$

or, equivalently,

$$\int_I^F L(x(t),\dot{x}(t);\Phi,A)dt = \text{extremal}. \quad (3.24)$$

Here $L(\cdot,\cdot;\Phi,A)$ is a Lagrangian of the Newtonian system (3.17) defined by

$$L(x(t),\dot{x}(t);\Phi,A) = (m/2)|\dot{x}(t)|^2 + eA(x(t),t)\cdot\dot{x}(t) - e\Phi(x(t),t). \quad (3.25)$$

Then Newton's equation of motion turns to be the Euler–Lagrange equation

$$\frac{d}{dt}\left[\frac{\partial L}{\partial \dot{x}(t)}\right]-\frac{\partial L}{\partial x(t)}=0. \tag{3.26}$$

Such a Newtonian system which admits the Lagrangian formalism as (3.17) I call a Lagrangian system.[6,7]

Though NSM has close correspondence to the Newtonian formalism of classical mechanics, as we have seen, it is also closely related to the Lagrangian formalism. Namely I have the following.

Theorem 3. The time-symmetric stochastic control problem (3.18) and (3.19) with the initial constraints (2.6) and (2.7) allows us to replace the control constraint (3.19), that is, Newton's equation of motion in a generalized sense, by the following variational constraint.

$$\begin{aligned}J[x;\Phi,A]&=\mathbb{E}\left[\int_I^F L\,(x(t,\omega),Dx(t,\omega),D_*x(t,\omega);\Phi,A\,)dt\right]\\&=\text{extremal.}\end{aligned} \tag{3.27}$$

Here

$$\begin{aligned}L\,(x(t,\omega),Dx(t,\omega),D_*x(t,\omega);\Phi,A\,)&=\tfrac{1}{2}[(m/2)|Dx(t,\omega)|^2+(m/2)|D_*x(t,\omega)|^2]\\&\quad+eA\,(x(t,\omega),t\,)\cdot\tfrac{1}{2}[Dx(t,\omega)+D_*x(t,\omega)]\\&\quad-e\Phi\,(x(t,\omega),t\,),\end{aligned} \tag{3.28}$$

is a natural extension of the notion of Lagrangian in classical mechanics (3.25).

Proof. Let $x'(t,\omega)=x(t,\omega)+\delta x(t,\omega)$, $I\leqslant t\leqslant F$, be a sample-wise variation of the sample path $x(t,\omega)$, $I\leqslant t\leqslant F$, with end point constraints $\delta x(I,\omega)=\delta x(F,\omega)=0$. Then I calculate the variation

$$\delta J[x;\Phi,A]=J[x';\Phi,A]-J[x;\Phi,A], \tag{3.29}$$

up to the first order in $\|\delta x\|=\max_{I\leqslant t\leqslant F}\{\mathbb{E}[|\delta x(t,\omega)|^2]\}^{1/2}$, obtaining

$$\begin{aligned}\delta J[x;\Phi,A]&=\mathbb{E}\left[\int_I^F m\tfrac{1}{2}(Dx(t,\omega)\cdot D\delta x(t,\omega)\right.\\&\quad\left.+D_*x(t,\omega)\cdot D_*\delta x(t,\omega))dt\right]\\&\quad+\mathbb{E}\left[\int_I^F eA\,(x(t,\omega),t\,)\cdot\tfrac{1}{2}(D\delta x(t,\omega)+D_*\delta x(t,\omega))dt\right]\\&\quad+\mathbb{E}\left[\int_I^F e\delta x(t,\omega)\cdot\text{grad}A\,(x(t,\omega,t\,)\right.\\&\quad\left.\times\tfrac{1}{2}[Dx(t,\omega)+D_*x(t,\omega)]dt\right]\\&\quad-\mathbb{E}\left[\int_I^F e\,\text{grad}\Phi\,(x(t,\omega),t\,)dt\right].\end{aligned} \tag{3.30}$$

Observing the properties

$$\begin{aligned}\mathbb{E}\left[\int_I^F f(x(t,\omega),t\,)D\delta x(t,\omega)dt\right]&=-\mathbb{E}\left[\int_I^F \delta x(t,\omega)D_*\,f(x(t,\omega),t\,)dt\right],\end{aligned} \tag{3.31}$$

$$\begin{aligned}\mathbb{E}\left[\int_I^F f(x(t,\omega),t\,)D_*\delta x(t,\omega)dt\right]&=-\mathbb{E}\left[\int_I^F \delta x(t,\omega)Df(x(t,\omega),t\,)dt\right],\end{aligned} \tag{3.32}$$

and

$$\begin{aligned}\tfrac{1}{2}(D+D_*)f(x(t,\omega),t\,)&=\left\{\frac{\partial}{\partial t}+\tfrac{1}{2}[Dx(t,\omega)+D_*x(t,\omega)]\cdot\text{grad}\right\}f(x(t,\omega),t\,),\end{aligned} \tag{3.33}$$

for any function f of position and time of class C^2,[3,11] I find

$$\begin{aligned}\delta J[x;\Phi,A]&=-\mathbb{E}\left[\int_I^F\left(m\tfrac{1}{2}(DD_*+D_*D)x(t,\omega)\right.\right.\\&\quad-e[\text{grad}\wedge A\,(x(t,\omega),t\,)]\cdot\tfrac{1}{2}[Dx(t,\omega)+D_*x(t,\omega)]\\&\quad\left.+e\,\text{grad}\Phi\,(x(t,\omega),t\,)+e\frac{\partial}{\partial t}A\,(x(t,\omega),t\,)\right)\\&\quad\left.\times\delta x(t,\omega)dt\right]+o(\|\delta x\|).\end{aligned} \tag{3.34}$$

By virtue of the variational constraint (3.27), the first order variation of $J[x;\Phi,A]$ must be zero for arbitrary sample-wise variation $\delta x(t,\omega)$, $I\leqslant t\leqslant F$. As the expectation $\mathbb{E}[\cdot]$ is a positive linear functional, this claims that

$$\begin{aligned}m\tfrac{1}{2}(DD_*+D_*D)x(t,\omega)&=-e\left\{\text{grad}\Phi\,[x(t,\omega),t\,]+\frac{\partial}{\partial t}A\,[x(t,\omega),t\,]\right\}\\&\quad+e\{\text{grad}\wedge A\,[x(t,\omega),t\,]\cdot\tfrac{1}{2}(D+D_*)x(t,\omega),\end{aligned} \tag{3.35}$$

for each time $t\in[I,F]$ with probability one. QED

Theorem 3 suggests to us the use of the notion of stochastic calculus of variations in NSM. It seems worthwhile to present a brief survey on the theory of stochastic calculus of variations in a compact form. This is done in the Appendix of the present paper.

4. EMERGENCE OF NSM

In the preceding sections I developed a general theory of NSM in a mathematical framework of the stochastic control theory. There, a class of time-symmetric stochastic control problems was proposed as a new representative of quantum mechanics. Evidently, with certain additional control constraints, those stochastic control problems were found to be equivalent to SWM.

Now, for the purpose of civilizing NSM in the realm of quantum mechanics, I shall verify some basic characters and specific features of NSM which can not be achieved by the other representatives of quantum mechanics, i.e., SWM, HMM, and FPI. To do so, I choose several topics of quantum mechanics which are hard to be investigated profoundly with the use of SWM, HMM, and FPI. Of course, there exist some topics of quantum mechanics which do not admit NSM but one or some of the other representatives, because

NSM is not the most general one. In any case we have to consider the complementarity structure of quantum mechanics (1.2) when we apply quantum mechanics to certain concrete physical problems in atomic scale.

As topics, I choose the following: Schrödinger's variational method of quantization, nonconservative quantum mechanics, instantons in vacuum tunneling phenomena, and Dirac monopoles.

A. Schrödinger's original quantization procedure revisited

In 1926 Schrödinger derived the famous eigenvalue problem

$$-(\hbar^2/2m)\,\mathrm{div}\,\mathrm{grad}u + Vu = Eu, \tag{4.1}$$

for a wavefunction $u(\cdot)\in L_2(\mathbb{R}^n)$, to characterize quantum mechanical stationary states of the Newtonian system (2.2).[15] He obtained Eq. (4.1) starting from the reduced Hamilton–Jacobi equation in classical mechanics equivalent to Newton's equation of motion (2.2),

$$(1/2m)|\,\mathrm{grad}W(x)|^2 + V(x) = E, \tag{4.2}$$

where $W: \mathbb{R}^n \to \mathbb{R}$ is an action function of class C^1 and E is the conserved energy of the system. By a substitution $W(\cdot) = \hbar \log v(\cdot)$, Eq. (4.2) becomes

$$(\hbar^2/2m)|\,\mathrm{grad}v(x)|^2/v^2(x) + V(x) = E. \tag{4.3}$$

Then he set up a variational problem

$$\delta J[v] = 0 \tag{4.4}$$

for a functional

$$J[v] = \int [(\hbar^2/2m)|\,\mathrm{grad}v(x)|^2/v^2(x) + V(x) - E\,]v^2(x)d^nx, \tag{4.5}$$

assuming the integral exists. He claimed it was not the classical problem (4.2) but the variational problem (4.4) and (4.5) which gave us correct mechanics in atomic scale. Evidently Eq. (4.4) led Schrödinger to Eq. (4.1). SWM was originated by such a variational method as (4.4) and (4.5).

Is his variational condition of quantization (4.4) equivalent to certain quantization conditions in the other representatives of quantum mechanics? Surely in NSM we have such a quantization condition.

By Theorem 2 we know that quantum mechanical stationary states are represented in NSM by optimal solutions to the time-symmetric stochastic control problem (3.5) and (3.6). As the stochastic differential equation (3.5) generates a Markov process with an invariant probability measure $p(x;V)\,d^nx$ on $\mathbb{R}^n$ such that,

$$-\mathrm{div}[b\,(b;V)\,p(x;V)] + (\hbar/2m)\,\mathrm{div}\,\mathrm{grad}p(x;V) = 0, \tag{4.6}$$

the control constraint (3.6) can be written in a form,

$$\int [(m/2)|b\,(x;V)|^2 + V(x) - E\,]\,p(x;V)d^nx = \text{extremal}. \tag{4.7}$$

This control constraint is equivalent to Schrödinger's variational condition of quantization (4.4) and (4.5) by virtue of Eq. (4.6). Thus, Schrödinger's monumental passage from the classical problem (4.2) to the variational problem (4.4) is justified as a quantization procedure within the realm of NSM.

B. Nonconservative quantum mechanics

Let us consider the quantization problem of a Newtonian nonconservative system in classical mechanics. The Newtonian nonconservative system is, in general, a Newtonian system, $x(\cdot): [I,F] \to \mathbb{R}^n$, which does not admit the Lagrangian and Hamiltonian formalisms. Time evolution of the system is given only by Newton's equation of motion,

$$m\ddot{x}(t) = F(x(t),\dot{x}(t),t), \tag{4.8}$$

where smoothness of the force $F: \mathbb{R}^n\times\mathbb{R}^n\times[I,F]\to\mathbb{R}^n$ is assumed. Clearly we can not adopt HMM, SWM, and FPI to quantize such a nonconservative system as (4.8). However, in NSM, one can construct nonconservative quantum mechanics with the help of the stochastic control theory. This is ensured by a fact that NSM has a close correspondence to the Newtonian formalism of classical mechanics.

According to the general theory of NSM developed in the preceding sections, quantum mechanics of the Newtonian nonconservative system (4.8) is given by the time-symmetric stochastic control problem.

$$dx(t,\omega) = b\,(x(t,\omega),t;F)dt + (\hbar/2m)^{1/2}dw(t,\omega), \tag{4.9}$$

where the control variable $b\,(\cdot,t;F)$ is controlled to satisfy a control constraint,

$$m\tfrac{1}{2}(DD_* + D_*D)x(t,\omega) = F\,(x(t,\omega),\tfrac{1}{2}(D + D_*)x(t,\omega),t\,), \tag{4.10}$$

for each time $t\in[I,F]$ with probability one, and initial constraints similar to (2.6) and (2.7). Although it may be difficult to solve directly the stochastic control problem (4.9) and (4.10), optimal solutions to this illustrate in principle the quantum mechanical time evolution of the Newtonian nonconservative system (4.8). Unfortunately, we can not verify the validity of the stochastic control problem (4.9) and (4.10) as a physically established candidate of nonconservative quantum mechanics in a systematic way. All we can do is to apply the present formalism (4.9) and (4.10) to a class of known Newtonian nonconservative systems and to clarify the physical validity of the results.

Here I consider the simplest class of Newtonian nonconservative systems such that,

$$m\ddot{x}(t) = -\beta\dot{x}(t) - \mathrm{grad}V(x(t)), \tag{4.11}$$

where β is a positive constant. Then I have the following.

Theorem 4. The time-symmetric stochastic control problem (4.9) and (4.10), in which the force F is given by the right hand side of Eq. (4.11), with the additional integrability constraints(2.15) and (2.16) is equivalent to a Cauchy problem for a nonlinear Schrödinger equation,

$$i\hbar\frac{\partial}{\partial t}\psi(x,t;\beta,V) = -(\hbar^2/2m)\,\mathrm{div}\,\mathrm{grad}\psi(x,t;\beta,V) + V(x)\psi(x,t;\beta,V) + (\beta\hbar/m)\arg[\psi(x,t;\beta,V)]\psi(x,t;\beta,V), \tag{4.12}$$

where arg[z] is an argument of $z\in\mathbb{C}$ (mod. 2π), with the initial condition (2.19).

Proof. The same technique as Nelson's in the case of the Newtonian conservative system (2.2) is also valid under the substitution,

$$V(\cdot)\rightarrow V(\cdot) + (\beta\hbar/m)S(\cdot,\cdot;\beta,V), \tag{4.13}$$

and this provides Eq. (4.12) directly because of the integrability constraint (2.15). QED

The nonlinear Schrödinger equation (4.12) has been carefully verified recently and found to produce physically meaningful results when applied to nonequilibrium quantum statistical mechanics.[16,17] This suggests to us, even in a restricted case, the validity of the stochastic control problem (4.9) and (4.10) as a representative of nonconservative quantum mechanics.

Furthermore, for the simplest class of Newtonian nonconservative systems as (4.11) I have the following

Theorem 5. The control constraint in Theorem 4,

$$m\tfrac{1}{2}(DD_* + D_*D)x(t,\omega) = -\beta\tfrac{1}{2}(D + D_*)x(t,\omega) - \operatorname{grad}V(x(t,\omega)), \tag{4.14}$$

for each time $t\in[I,F]$ with probability one, is equivalent to the following control constraint with "discount".

$$\mathbb{E}\left[\int_I^F e^{+\beta(t-I)}\left[\tfrac{1}{2}[(m/2)|Dx(t,\omega)|^2 + (m/2)|D_*x(t,\omega)|^2] - V(x(t,\omega))\right]dt\right] = \text{extremal}. \tag{4.15}$$

Proof. From a viewpoint of the theory of stochastic calculus of variations developed in the appendix, Eq. (4.14) is nothing but the Euler–Lagrange equation in a generalized sense (A7) for the stochastic variational problem (4.15). Then, the equivalence in question is ensured by Theorem A. QED

C. Instantons in vacuum tunneling phenomena

Consider the Newtonian conservative system (2.2) in which the potential energy of the system $V(\cdot)$ has several minima, $x_a, x_b,\cdots,x_z\in\mathbb{R}^n$, say, such that $V(x_a) = V(x_b) = \cdots = V(x_z)$. In classical mechanics, they are equal candidates of classical vacuum states of the system because they give the lowest energy configurations. Such classical vacua as x_a's are stable as long as classical mechanics is concerned. However, they are rendered unstable in quantum mechanics by tunnel effects. How can one visualize such tunneling processes and in which manner can one describe the quantum mechanical decay of classical vacua? HMM and SWM are not powerful in such analyses. The use of FPI together with the analytic continuation of time was proposed.[18,19] Here I shall investigate the problem in question from the stochastic control theoretical point of view of NSM.[20]

Following the results obtained in Sec. 3, NSM claims that the quantum mechanical vacuum state (i.e., the lowest energy stationary state) of the Newtonian conservative system (2.2) is an optimal solution to the time-symmetric stochastic control problem (3.5) and (3.6) for the smallest admissible value of E. The results obtained in subsection 4A teach us that such an optimal solution is obtained with the help of the eigenvalue problem (4.1). Let $u_0(\cdot)\in L_2(\mathbb{R}^n)$ be a positive eigenfunction of Eq. (4.1) associated with the lowest eigenvalue E_0. Then the control variable

$$b_0(\cdot;V) = (\hbar/m)\operatorname{grad}\log u_0(\cdot), \tag{4.16}$$

solves optimally the time-symmetric stochastic control problem (3.5) and (3.6). Therefore, the quantum mechanical time evolution of the system in the vacuum state is visualized as a stationary random process in $\mathbb{R}^n$ generated by the stochastic differential equation of Itô type,

$$dx(t,\omega) = b_0(x(t,\omega);V)dt + (\hbar/2m)^{1/2}dw(t,\omega). \tag{4.17}$$

This is a Markov process with an invariant probability measure $|u_0(x)|^2d^nx$. In NSM I can refer to Eq. (4.17). It provides us with a powerful mathematical tool in investigating the quantum mechanical instability of classical vacua as pointed out by Jona-Lasinio.[21]

According to the general theory of stochastic differential equations,[10] Eq. (4.17) generates a stationary Markovian random flow $\mathscr{X}^r(\omega):\mathbb{R}^n\rightarrow\mathbb{R}^n$, $r\in[0,\infty)$, such that

$$\mathscr{X}^{t-s}(\omega)x(s,\omega) = x(t,\omega), \tag{4.18}$$

for $I\leqslant s<t\leqslant F$, with probability one. If the classical vacua x_a's are (not) asymptotically stable under this flow $\mathscr{X}^r(\omega)$, they are (not) stable in quantum mechanics. The characteristic of the stationary Markovian random flow $\mathscr{X}^r(\omega)$ is mostly illustrated by the transition law

$$p^r(d^nx,y) = \operatorname{Prob}(\{\mathscr{X}^r(\omega)y\in d^nx\}). \tag{4.19}$$

Assume it has a density $p^r(x,y)$ such that $p^r(x,y)d^nx = p^r(d^nx,y)$. By Eq. (4.17) it follows immediately that the density $p^r(\cdot,y)\in L_1(\mathbb{R}^n)$ is an elementary solution to the Fokker–Planck equation (2.17) in which $b(\cdot,t;V)$ is replaced by $b_0(\cdot;V)$. In other words, the transition probability density $p^r(x,y)$ is a solution to the Cauchy problem

$$\frac{\partial}{\partial r}p^r(x,y) = -\operatorname{div}(b_0(x;V)p^r(x,y)) + (\hbar/2m)\operatorname{div}\operatorname{grad}p^r(x,y), \tag{4.20}$$

with an initial condition

$$p^0(x,y) = \delta_y(x), \tag{4.21}$$

where $\delta_y(\cdot)$ denotes a point mass (Dirac distribution) located at $y\in\mathbb{R}^n$.

Firstly, I shall discuss the quantum mechanical instability of the classical vacua x_a's qualitatively. By a symmetry consideration it is easy to find that x_a's are also stationary point of the vector field $b_0(\cdot;V):\mathbb{R}^n\rightarrow\mathbb{R}^n$ such that $b_0(x_a;V) = 0$ and so on. Let ϵ be a sufficiently small position number and $B(x_a,\epsilon)\subset\mathbb{R}^n$ be a ball of radius ϵ centered at x_a. Then $b_0(\cdot;V) = 0$ approximately in $B(x_a,\epsilon)$, and Eq. (4.17) becomes,

$$dx(t,\omega) = (\hbar/2m)^{1/2}dw(t,\omega), \tag{4.22}$$

approximately in $B(x_a,\epsilon)$. As the random flow $\mathscr{X}^r(\omega)$ can be approximated in $B(x_a,\epsilon)$ by the Wiener flow $\mathscr{W}^r(\omega):\mathbb{R}^n\rightarrow\mathbb{R}^n$ such that $\mathscr{W}^{t-s}(\omega)\,w(s,\omega) = w(t,\omega)$, $t>s$, one finds

$$\limsup_{r\to\infty} \text{Prob}(\{\mathscr{X}^r x_a \in B(x_a,\epsilon)\})$$
$$= \limsup_{r\to\infty} \text{Prob}(\{\mathscr{W}^r x_a \in B(x_a,\epsilon)\})$$
$$= 0. \tag{4.23}$$

This claims that the classical vacua x_a's are not asymptotically stable under the random flow $\mathscr{X}^r(\omega)$ and so they are rendered unstable in quantum mechanics. Such a direct qualitative analysis of the quantum mechanical instability of classical vacua is possible only within the realm of NSM.

Next, for the purpose of investigating the quantum mechanical decay of the classical vacua x_a's quantitatively, I shall compute the transition probability density $p^r(x,x_a)$. The Fokker–Planck equation (4.20) is considered in $L_2(\mathbb{R}^n) = L_2(\mathbb{R}^n, d^n x)$. However it is convenient and natural to consider it in $L_2(\mathbb{R}^n, |u_0(x)|^2 d^n x)$ because the random flow $\mathscr{X}^r(\omega)$ leaves the measure $|u_0(x)|^2 d^n x$ invariant. In fact, there exists a unitary transformation $U: L_2(\mathbb{R}^n) \to L_2(\mathbb{R}^n, |u_0(x)|^2 d^n x)$ under which Eqs. (4.20) and (4.21) are transformed in the forms

$$-\hbar \frac{\partial}{\partial r} q^r(x,x_a) = [-(\hbar^2/2m)\,\text{div grad} + V(x) - E_0]q^r(x,x_a), \tag{4.24}$$

and

$$q^0(x,x_a) = \delta_{x_a}(x), \tag{4.25}$$

where $q^r(\cdot,x_a) = Up^r(\cdot,x_a) \in L_2(\mathbb{R}^n, |u_0(x)|^2 d^n x)$.[22] A solution to the Cauchy problem (4.24) and (4.25) is given by the Feynman–Kac formula.[23]

$$q^r(x,x_a) = \int \exp\left\{-\hbar^{-1}\int_0^r [V(\omega_t) - E_0]dt\right\} \text{Prob}^w(d\omega). \tag{4.26}$$

Here $\text{Prob}^w(\cdot)$ denotes a Wiener measure with diffusion constant $\hbar/2m$. Support of the Wiener measure $\text{Prob}^w(\cdot)$ is concentrated on continuous paths ω's in $\mathbb{R}^n$ with endpoints $\omega_0 = x_a$ and $\omega_r = x$. Equation (4.26), when transformed to $L_2(\mathbb{R}^n)$ by U^{-1}, gives us the Prokhorov formula,[24,25] though I do not present it here.

By virtue of Eq. (4.26), I conclude that the quantum mechanical decay of the classical vacua x_a's may occur along any continuous path ω started from x_a with probability,

$$\exp\left\{-\hbar^{-1}\int_0^r [V(\omega_t) - E_0]dt\right\} \text{Prob}^w(d\omega). \tag{4.27}$$

Let us make use of a heuristic notion of the Wiener measure

$$\text{Prob}^w(d\omega) = N^{-1}\exp\left[-h^{-1}\int_0^r (m/2)|\dot\omega_t|^2 dt\right]\text{`}d\omega\text{'}, \tag{4.28}$$

where the equality holds only when one makes a nonstandard analysis consideration of the infinite normalization factor N and the nonstandard Lebesgue measure '$d\omega$'.[17] Of course, Eq. (4.28) should be understood that the standard part[26] of the right hand side is equal to the Wiener measure Prob^w. Then Eq. (4.27) becomes

$$\exp\left\{-h^{-1}\int_0^r [(m/2)|\dot\omega_t|^2 + V(\omega_t)]dt\right\} \cdot \exp(E_0 r/h)\text{`}d\omega\text{'}, \tag{4.29}$$

from which I find it most probable that the quantum mechanical decay of the classical vacuum x_a occurs along a path $x_{in}(\cdot): [0,r] \to \mathbb{R}^n$ of class C^1 with end points $x_{in}(0) = x_a$ and $x_{in}(r) = x$ which minimizes the integral

$$\int_0^r [(m/2)|\dot\omega_t|^2 + V(\omega_t)]dt. \tag{4.30}$$

This is nothing but a Euclidean (i.e., elliptic) action integral constructed from the normal action integral of the Newtonian conservative system (2.2) by an analytic continuation of time $t \to it$. The path $x_{in}(\cdot)$, along which the classical vacuum x_a decays most probably, thus manifests the quantum mechanical tunneling process approximately and called "instanton."[20]

It is worthwhile to notice that the present probability theoretical consideration of the instanton in vacuum tunneling phenomena plays an important role in investigating the quantum theoretical vacuum structure of non-Abelian gauge fields in quantum chromodynamics (QCD).[27,28]

D. Dirac monopoles

As the last exposition of the emergence of NSM, I shall show here that a topological study of NSM gives us, quite naturally, the notion of magnetic monople. It will be clarified that quantum mechanics, in its form of NSM, admits the incorporation of a new degree of freedom of magnetic monopoles. It was Dirac who developed a general theory of magnetic monopoles in a quantum mechanical context.[29] So I call them simply "Dirac monopoles" hereafter.

Consider the Newtonian conservative system (2.2). As I emphasized in Sec. 2, quantum mechanics of the Newtonian system (2.2) was obtained in NSM as an optimal solution to the time-symmetric stochastic control problem (2.4), (2.5), (2.6), and (2.7). In a restricted case, this coincided with SWM, namely, the time-symmetric stochastic control problem in question was found to be equivalent to the Cauchy problem for the Schrödinger equation (2.18) if the additional integrability constraint (2.15) was imposed. However, from the point of view of NSM, it is not of necessity in general to impose such an integrability constraint. NSM has certainly the capacity of describing some unusual physical situations in atomic scale which never appeared in classical mechanics. What kind of new degree of freedom does NSM admit in its form without the integrability constraint? To find it I need a simple topological study of the control variable $b(\cdot,t;V)$.

Let us introduce a time-dependent vector field,

$$v(\cdot,t;V) = \tfrac{1}{2}[b(\cdot,t;V) + b_*(\cdot,t;V)], \tag{4.31}$$

for each time $t \in [I,F]$. It generates the mean velocity in such a way that

$$v(x(t,\omega),t;V) = \tfrac{1}{2}(D + D_*)x(t,\omega), \tag{4.32}$$

with probability one. Fix a point in space, say $R \in \mathbb{R}^n$, and call it a reference point. Then I define a function $Q(\cdot,\cdot;V): \mathbb{R}^{an} \times [I,F] \to \mathbb{R}$ by a line integral

$$Q(x,t;V) = (m/\hbar) \int_R^x v(z,t;V)\cdot dz, \quad (4.33)$$

where the integral is performed along a curve of class C^1 in $\mathbb{R}^n$, say Γ, connecting R and x. Clearly, such a function as (4.33) can not have a definite value. Because we have no longer any integrability constraint, Eq. (4.33) depends on the choice of Γ. Integrations along different curves define different values of $Q(x,t;V)$. It is a nonintegrable function of position for each time $t\in[I,F]$. In general, $Q(z,t;V)$ does not depend on all of the possible curves but some of them. By the notion of homotopy class of $Q(x,t;V)$, I denote a class of curves of class C^1 which give the same values to the integral (4.33).

Now I define a nonintegrable wavefunction by

$$\psi(\cdot,t;V) = p(\cdot,t;V)^{1/2} \exp[iQ(\cdot,t;V)], \quad (4.34)$$

where

$$mv(\cdot,t;V) = \hbar \operatorname{grad} Q(\cdot,t;V), \quad (4.35)$$

holds for each time $t\in[I,F]$. Just following the same procedure as the case with the integrability constraint (2.15), I find that the nonintegrable wavefunction (4.34) also satisfies the Schrödinger equation (2.18). The crucial point is that the nonintegrability of the wavefunction is generally admitted within the realm of NSM as a consequence of the mathematical structure involved. It is not introduced in the theory "by hand," but it has been in the theory.

The concept of nonintegrable wavefunction was the very starting point of the incorporation of Dirac monopoles in quantum mechanics.[29] Therefore, I conclude that NSM has a mathematical structure which admits naturally the existence of Dirac monopoles, though I do not sketch here why the nonintegrability of wavefunction results in Dirac monopoles. However it seems worthwhile to notice an important fact from the present stochastic control theoretical point of view of NSM. The nonintegrability of wavefunction does not enter the theory, even when the integrability constraint is no longer assumed, if wavefunctions are initially integrable. The time-symmetric stochastic control problem (2.4), (2.5), (2.6), and (2.7) always admits an optimal integrable solution if the initial constraint (2.7) is integrable. NSM claims thus physically that there will be no chance to find out Dirac monopoles if there are no Dirac monopoles initially.

5. CLASSICAL LIMIT OF QUANTUM MECHANICS

In this section I will show how classical mechanics is realized within the realm of the present stochastic control theoretical formulation of NSM as a limit of quantum mechanics when $\hbar$ tends to zero.

In SWM, classical mechanics is obtained in the limit $\hbar\to 0$ because the lowest order term in the asymptotic expansion of the Schrödinger equation coincides with the Hamilton–Jacobi equation.[30] In HMM, Heisenberg's equation of motion for noncommutative canonical variables tends to Hamilton's equation of motion for ordinary (commuting) canonical variables in the same limit. The stationary phase approximation with $\hbar\to 0$ of path integrals recovers the Lagrangian formalism of classical mechanics in FPI. How about in NSM?

Let us start out with the time-symmetric stochastic control problem (3.18) and (3.19). An optimal solution to it is a representative of the quantum mechanical time evolution of the Newtonian system (3.17) with a charge degree of freedom. By Theorem 3 we know that the control constraint (3.19) is equivalent to the variational constraint (3.27). I shall investigate the limit behavior of the solution to the time-symmetric stochastic control problem (3.18) and (3.27) for small $\hbar$, hoping it provides us classical mechanics. To do so, it is convenient to perform asymptotic expansions in powers of $\hbar$,[8] namely, for sufficiently small $\hbar$, look for an optimal solution of the form

$$x(t,\omega) = z(t) + \hbar y(t,\omega) + o(\hbar), \quad (5.1)$$

where the zeroth order term $z(\cdot)$ is not a random process but an ordinary function of time of class C^1. Correspondingly, the mean forward and backward derivatives become

$$Dx(t,\omega) = \dot z(t) + \hbar Dy(t,\omega) + o(\hbar), \quad (5.2)$$

$$D_* x(t,\omega) = \dot z(t) + \hbar D_* y(t,\omega) + o(\hbar), \quad (5.3)$$

respectively. Then I find an asymptotic expansion of the variational constraint (3.27),

$$\mathrm{E}\left[\int_I^F L(z(t),\dot z(t);\Phi,A)dt + o(\hbar^0)\right] = \int_I^F L(z(t),\dot z(t);\Phi,A)dt + o(\hbar^0) = \text{extremal}, \quad (5.4)$$

where $L(\cdot,\cdot;\Phi,A)$ is nothing but the Lagrangian in classical mechanics given by Eq. (3.25). As the variational constraint (5.4) must be satisfied in each power of $\hbar$, the zeroth order term $z(\cdot)$ of the optimal solution (5.1) is obtained by an ordinary (nonrandom) variational principle,

$$\int_I^F L(z(t),\dot z(t);\Phi,A)dt = \text{extremal}. \quad (5.5)$$

This is the very Lagrangian formalism of classical mechanics for the Newtonian system (3.17). In NSM, classical mechanics is thus realized by the lowest order term of the asymptotic expansion in powers of $\hbar$ of the optimal solution to the time-symmetric stochastic control problem (3.18) and (3.27).

The above observation of the classical limit of quantum mechanics within the realm of NSM suggests to us that the passage from classical mechanics to quantum mechanics in NSM is conceptually simple and natural. Quantum mechanics is a natural extension of classical mechanics. This is what I want to emphasize from a point of view of the optimal control theory.

6. A SHORT CONCLUDING REMARK

In the present paper I have developed a time-symmetric stochastic control theory as one of the representatives of quantum mechanics. I do not repeat here the results obtained. I want to emphasize simply that I made an effort to clarify many facts which suggest the validities of Eq. (1.2) and of civilizing NSM in the nation of quantum mechanics. I myself believe that the present stochastic control theoretical formulation of quantum mechanics will provide a new viewpoint in understanding Nature in atomic scale.

Nature controls everything, even in atomic scale, as Buddha recognized a long long time ago.

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APPENDIX: STOCHASTIC CALCULUS OF VARIATIONS

This appendix is devoted to an exposition of the theory of stochastic calculus of variations in a compact form.

Let $L\mathbb{R}^n\times\mathbb{R}^n\times\mathbb{R}^n\times[I,F]\to\mathbb{R}^n$ be a function of class C^1, call it Lagrangian in a generalized sense, and $x(t,\omega)$, $I\leqslant t\leqslant F$, be a random process defined on the probability space $(\Omega,\mathscr{D}(\text{Prob}),\text{Prob})$ such that the mean forward and backward derivatives $Dx(t,\omega)$ and $D_* x(t,\omega)$ exist in $L_1(\Omega,\text{Prob})$ for each time $t\in[I,F]$ and are continuous functions of time. Almost all sample paths are assumed to be continuous. Nelson called such a random process an (S1) process.[3] By the notion of action integral in a generalized sense, I denote a functional,

$$J[x]=\mathbb{E}\left[\int_I^F L\,(x(t,\omega),Dx(t,\omega),D_* x(t,\omega),t\,)dt\right]. \qquad \text{(A1)}$$

A functional $J[\cdot]$: $\Omega\to\mathbb{R}$ is differentiable if,

$$\begin{aligned}\delta J[x]&=J[x+\delta x]-J[x]\\ &=dJ[\delta x]+R[\delta x,x],\end{aligned} \qquad \text{(A2)}$$

where $dJ[\cdot]$ is a linear functional of δx and $R[\delta x,x]=o(\|\delta x\|)$. The linear part $dJ[\cdot]$ is called a (functional) derivative of $J[\cdot]$. Then I have the following.

Theorem A. The action integral (A1) is differentiable and has a derivative

$$\begin{aligned}dJ[\delta x]=\mathbb{E}\Bigg[\int_I^F\Bigg\{&\frac{\partial L}{\partial x(t,\omega)}-D\left[\frac{\partial L}{\partial D_* x(t,\omega)}\right]-D_*\left[\frac{\partial L}{\partial Dx(t,\omega)}\right]\Bigg\}\\ &\times\delta x(t,\omega)dt+\left[\frac{\partial L}{\partial D_* x(t,\omega)}+\frac{\partial L}{\partial Dx(t,\omega)}\right]\cdot\delta x(t,\omega)\Bigg|_I^F\Bigg].\end{aligned} \qquad \text{(A3)}$$

Proof. Straightforward calculations as in the case of Theorem 3 give

$$\begin{aligned}\delta J[x]=\mathbb{E}\Bigg[\int_I^F\Bigg(&\frac{\partial L}{\partial x(t,\omega)}\cdot\delta x(t,\omega)+\frac{\partial L}{\partial Dx(t,\omega)}\cdot D\delta x(t,\omega)\\ &+\frac{\partial L}{\partial D_* x(t,\omega)}\cdot D_*\delta x(t,\omega)\Bigg)dt\Bigg]+o(\|\delta x\|).\end{aligned} \qquad \text{(A4)}$$

By Nelson's rule in stochastic calculus,[3] I have

$$\begin{aligned}\mathbb{E}\left[\frac{\partial L}{\partial Dx(t,\omega)}\cdot D\delta x(t,\omega)\right]&=-\mathbb{E}\left[\delta x(t,\omega)\cdot D_*\left(\frac{\partial L}{\partial Dx(t,\omega)}\right)\right]\\ &\quad+\frac{d}{dt}\mathbb{E}\left[\frac{\partial L}{\partial Dx(t,\omega)}\cdot\delta x(t,\omega)\right],\end{aligned} \qquad \text{(A5)}$$

and,

$$\begin{aligned}\mathbb{E}\left[\frac{\partial L}{\partial D_* x(t,\omega)}\cdot D_*\delta x(t,\omega)\right]&=-\mathbb{E}\left[\delta x(t,\omega)\cdot D\left(\frac{\partial L}{\partial D_* x(t,\omega)}\right)\right]\\ &\quad+\frac{d}{dt}\mathbb{E}\left[\frac{\partial L}{\partial D_* x(t,\omega)}\cdot\delta x(t,\omega)\right],\end{aligned} \qquad \text{(A6)}$$

which admit us to obtain the desired result. QED

This theorem claims that an extremal constraint $dJ[\delta x]=0$ with respect to a sample-wise variation $\delta x(t,\omega)$, $I\leqslant t\leqslant F$, such that $\delta x(I,\omega)=\delta x(F,\omega)=0$ is equivalent to a constraint

$$D\left[\frac{\partial L}{\partial D_* x(t,\omega)}\right]+D_*\left[\frac{\partial L}{\partial Dx(t,\omega)}\right]-\frac{\partial L}{\partial x(t,\omega)}=0, \qquad \text{(A7)}$$

for each time $t\in[I,F]$ with probability one. I shall call Eq. (A7) the Euler–Lagrange equation in a generalized sense. It is a natural extension of the Euler–Lagrange equation in ordinary calculus of variations.

For example, in ordinary calculus of variations, a path of class C^2 with minimum length, $x(\cdot)$:$[I,F]\to\mathbb{R}^n$, is given by a solution to the variational problem $\delta j[x]=0$ (or $dj[x]=0$) for a functional

$$j[x]=\int_I^F|\dot{x}(t)|dt. \qquad \text{(A8)}$$

Correspondingly, in stochastic calculus of variations, an (S1) process with minimum "length" $x(t,\omega)$, $I\leqslant t\leqslant F$, should be defined by a solution to the stochastic variational problem $\delta j_s[x]=0$ (or $dj_s[x]=0$) for a functional

$$j_s[x]=\mathbb{E}\left[\tfrac{1}{2}\int_I^F[|Dx(t,\omega)|+|D_* x(t,\omega)|]dt\right]. \qquad \text{(A9)}$$

The minimum of $j_s[\cdot]$ is achieved by stationary diffusion processes

$$x(t,\omega)=c_0+v_0t+\sigma_0w(t,\omega),\quad I\leqslant t\leqslant F, \qquad \text{(A10)}$$

for various values of constant vectors c_0,v_0, and constant scalar σ_0.

The present theory of stochastic calculus of variations can be used to systematically characterize a certain class of random processes and will open an interesting field of mathematical research, though it is beyond the scope of the present paper.

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A multidimensional extension of the combinatorics function technique. I
Linear and homogeneous partial difference equations

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This paper is aimed at series solutions of physical phenomena that are described by linear homogeneous differential equations, like the Schrödinger differential equation. Series solutions to such equations, when they exist, lead to multidimensional, linear, and homogeneous recurrence relations among the expansion coefficients. The physical constraints imposed on the solutions of an ordinary differential equation (in the case of the Schrödinger equation that would be on the wavefunctions) then lead to a set of "initial values" on the expansion coefficients. The consistency of the initial values with the recurrence relation or partial difference equation (PDE) is one of the major problems in such cases. Until now, there was no systematic way of obtaining the solution of a PDE in terms of the initial values, and no systematic technique dealing with the consistency check. In this paper, we have been able to solve both of these problems by a natural extension of the combinatorics function technique developed by Antippa and Phares for one-dimensional linear recurrence relations.

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I. INTRODUCTION

This paper is the first in a series aimed at an exact analytic solution of the nonrelativistic Schrödinger equation with central potentials. Our immediate goal is the general power type confinement potential whose exact solution is very well known for the harmonic case and has been recently obtained for the linear potential.[1–3] The new mathematical method that ultimately lead to the construction of the linear potential wavefunctions and eigenenergies is the combinatorics function technique (CFT). The CFT method, which has been discovered by Antippa and Phares,[4–6] enables one to write down the explicit solution of any one-dimensional linear recurrence relation in a noniterative fashion. Here, we develop the previously nonexistent theory of the most general multidimensional, linear, and homogeneous recurrence relation, also referred to as partial difference equation.

Partial difference equations[7] (PDE) arise when one attempts power series solutions to partial differential equations. Consider the following homogeneous and linear partial differential equation

$$L\psi(x_1,x_2,\ldots,x_i,\ldots)=0. \tag{1.1}$$

Here L stands for a linear differential operator acting on the multivariable function ψ. One can think of Eq. (1.1) as being the Schrödinger differential equation, and ψ as the wavefunction of a multiparticle system, where the x_i stand for an appropriate system of generalized coordinates. Assuming the existence of a series solution to Eq. (1.1) in the form

$$\psi=\sum_{m_i}B(m_1,m_2,\ldots,m_i,\ldots)(x_1)^{m_1}(x_2)^{m_2}\ldots(x_i)^{m_i}\ldots, \tag{1.2}$$

and replacing ψ by its series (1.2) in Eq. (1.1), the expansion coefficients B are found to satisfy a linear and homogeneous recurrence relation or PDE,

$$P(\mathbf{E})\,B(\mathbf{M})=0. \tag{1.3}$$

$\mathbf{M}$ stands for the set of values $\{m_1,m_2,\ldots,m_i,\ldots\}$ and P is a polynominal operator that depends on the set $\mathbf{E}$ of operators $E_1,E_2,\ldots,E_i,\ldots$. Each individual operator, say E_i, when acting on the coefficient function F will produce a shift in the variable m_i, according to

$$E_i\,B(m_1,\ldots,m_i,\ldots)=B(m_1,\ldots,m_i+1,\ldots). \tag{1.4}$$

The inverse operation E_i^{-1}, on the other hand, will produce the opposite shift, i.e.,

$$E_i^{-1}B(m_1,\ldots,m_i,\ldots)=B(m_1,\ldots,m_i+1,\ldots). \tag{1.5}$$

A typical term in the polynominal operator $P(\mathbf{E})$ is of the form $(\Pi_i\,E_i^{\alpha_i})$ where α_i may be any integer.

As an example, let us consider a two-variable function $B(m_1,m_2)$ that satisfies the partial difference equation

$$f_1B(m_1,m_2)+f_2B(m_1+2,m_2-1)+f_3B(m_1-4,m_2+2)=0. \tag{1.6}$$

Then,

$$P(E_1,E_2)=f_1+f_2E_1^2E_2^{-1}+f_3E_1^{-4}E_2^2. \tag{1.7}$$

Coefficients f_1, f_2, and f_3 need not be constant and may very well depend on m_1 and m_2. Equation (1.6) is meaningless unless one specifies a certain set of initial values of the function. In general not any set of initial values is necessarily consistent with the given PDE. These initial values will be called boundary conditions imposed on ψ.

A special case of Eq. (1.1) is the one-variable (or one-dimensinal) equation, which is most commonly called a homogeneous finite-difference equation[7],

$$P(E_1)B(m_1)=0. \tag{1.8}$$

The formal solution of such an equation was obtained a few years ago[4–6] by expressing $B(m_1)$ in terms of initial values corresponding to arguments of B less than m_1 (boundary conditions at the "lower end"),[4] or greater than m_1 (boundary conditions at the "upper end").[8] In those two cases, the boundary conditions are always consistent with the finite-difference equation. Then, this original work was generalized in two directions: (i) One of us (AJP) obtained the solution of the inhomogeneous equation associated with Eq. (1.8), by fixing the boundary conditions either at the "lower end" or at the "upper end".[5] (ii) Antippa extended the results of Refs. 4 and 8 to mixed boundary conditions.[6] In this latter case, Antippa based his solution on a discrete path approach to the problem, and found that the boundary conditions are not always consistent with the finite-difference equation (1.8). He also discovered in this particular case a systematic way of dealing with the consistency problem.

This paper presents a method for obtaining the formal solution of the more general PDE of the form given by Eq. (1.3). In one-dimension it reduces to the method used by Antippa[6] from which it is possible to recover the earlier results on bondary conditions either at the "lower end" or the "upper end".[4,8] The CFT concepts of "partitions" of a line element[4,5,8] and "discrete paths" in one-dimension[6] are very simply extended in n dimensions, thus leading to the formal solution of Eq. (1.3) for a still unspecified set of initial values.

II. DISCRETE PATHS AND COMBINATORICS FUNCTIONS

The solution of linear and homogeneous partial difference equations can be arrived at rather intuitively and rapidly. Our choice is to develop the subject with the same mathematical rigor and precision of language as done for one-dimensional recurrence relations.[4] The approach followed in Ref. 4 will be most illuminating and helpful.

A. Restricted discrete paths in an n-dimensional Euclidean space

Consider an n-dimensional Euclidean space. With every point in this space of coordinates $(m_1,m_2,...,m_n)$, one associates vector $\mathbf{M}$ whose components are $(m_1,m_2,...,m_n)$. Since there is a one-to-one correspondence between point $\mathbf{M}$ and vector $\mathbf{M}$ we will be using a loose language referring to M as either the point or its associated vector.

From point M only N discrete displacements or *steps* are allowed. These steps are represented by a set $\mathscr{A}$ of N vectors,

$$\mathscr{A} = \{\mathbf{A}_1,\mathbf{A}_2,...,\mathbf{A}_N\}, \tag{2.1}$$

so that leaving point M one can only reach points $\mathbf{M}-\mathbf{A}_1,\mathbf{M}-\mathbf{A}_2,...,$ and $\mathbf{M}-\mathbf{A}_N$, following discrete "backward" steps.

One also considers a set $\mathscr{J}$ of points in this space (in infinite or infinite number) that one refers to as *boundary points* represented by vectors $J_1,J_2,...,J_l,...,$ thus

$$\mathscr{J} = \{J_1,J_2,...,J_l,...\}. \tag{2.2}$$

A restricted discrete path is said to exist between point M and one of the boundary points, J, when it is possible to reach J following successive "backward"steps such that no intermediate point is a boundary point. If ω is the number of "forward" steps linking J to M, then

$$\mathbf{M}-\mathbf{J} = \sum_{i=1}^{\omega} \boldsymbol{\delta}_i \quad \text{and} \quad \boldsymbol{\delta}_i \in \mathscr{A}. \tag{2.3}$$

Two consecutive points $\mathbf{S}_{i-1}$ and $\mathbf{S}_i$ are then related according to

$$\mathbf{S}_i - \mathbf{S}_{i-1} = \boldsymbol{\delta}_i, \tag{2.4}$$

and the ordering of the intermediate points on the path is from $\mathbf{J}$ to $\mathbf{M}$, or

$$\mathbf{S}_0 = \mathbf{J} \quad \text{and} \quad \mathbf{S}_\omega = \mathbf{M}. \tag{2.5}$$

Since none of the intermediate points on the path may be one of the boundary points,

$$\mathbf{S}_i \notin J \quad \text{for} \quad i\neq 0. \tag{2.6}$$

In general, there may be more than one path connecting $\mathbf{J}$ to $\mathbf{M}$ into ω steps. To distinguish among different paths having the same number of steps we use the label q,

$$q = 1,2,...q_{\max}(\omega). \tag{2.7}$$

Here $q_{\max}(\omega)$ is the number of distinct paths connecting $\mathbf{J}$ to $\mathbf{M}$ into ω steps. With these definitions the (ωq)th path is isomorphic to the "ordered" set

$$\Delta_{\omega q} = \{\boldsymbol{\delta}_1,\boldsymbol{\delta}_2,...,\boldsymbol{\delta}_\omega\}. \tag{2.8}$$

By "ordered" set we mean that a different ordering of the $\boldsymbol{\delta}$'s, corresponding to another possible restricted path and, therefore, to another value of the label q, leads to a different set.

Let $\mathscr{M}$ be the set of *all* points $\mathbf{M}$ in space that do not have the following property:

There exists at least one path reaching point $\mathbf{M}$ by successive discrete steps belonging to $\mathscr{A}$ containing no boundary points belonging to $\mathscr{J}$. For such a set $\mathscr{M}$, the set $\mathscr{J}$ is called a "full boundary" of $\mathscr{M}$ with respect to $\mathscr{A}$.

Theorem:1 Let $\mathscr{J}_1$ and $\mathscr{J}_2$ be two full boundary sets of $\mathscr{M}$. Then $\mathscr{J}_1\cap\mathscr{J}_2$ is a full boundary $\mathscr{M}$ and no restricted path is possible connecting any element of $\mathscr{J}_1$ or $\mathscr{J}_2$, not belonging to $\mathscr{J}_1\cap\mathscr{J}_2$, to any element of $\mathscr{M}$.

Proof: Consider an element $\mathbf{J}_1$ of set $\mathscr{J}_1$ not belonging to the intersection $\mathscr{J}_1\cap\mathscr{J}_2$. Then $\mathbf{J}_1$ is not an element of $\mathscr{J}_2$. Since $\mathscr{J}_2$ is a full boundary of $\mathscr{M}$ and $\mathbf{J}_1$ does not belong to $\mathscr{J}_2$, then no restricted path is possible connecting $\mathbf{J}_1$ to any point $\mathbf{M}$ of set $\mathscr{M}$. The same is true for any element $\mathbf{J}_2$ of set $\mathscr{J}_2$ not belonging to $\mathscr{J}_1\cap\mathscr{J}_2$. Thus, only points that *effectively* generate $\mathscr{M}$ belong to the intersection $\mathscr{J}_1\cap\mathscr{J}_2$, and consequently $\mathscr{J}_1\cap\mathscr{J}_2$ is a full boundary of $\mathscr{M}$.

A direct consequence of this theorem is the existence of one and only one "minimal full boundary" $\mathscr{J}$ to set $\mathscr{M}$ for which each and every element can be connected to at least one element of $\mathscr{M}$ by at least one restricted path. Indeed, assume that there exist two minimal full boundary sets $\mathscr{J}'$ and $\mathscr{J}''$, and call $\mathscr{J}'_a$ and $\mathscr{J}''_a$ the part of $\mathscr{J}'$ and $\mathscr{J}''$, respectively, not included in $\mathscr{J}'\cap\mathscr{J}''$. Then, according to the definition of a minimal full boundary and Theorem 1, $\mathscr{J}'$ and $\mathscr{J}''$ must necessarily be empty, thus

$$\mathscr{J}'\cap\mathscr{J}'' = \mathscr{J}' \text{ and } \mathscr{J}'\cap\mathscr{J}'' = \mathscr{J}'' \text{ or } \mathscr{J}' = \mathscr{J}''.$$

We have thus established that, for a nonempty set $\mathscr{M}$ and a given set $\mathscr{A}$ of displacement vectors, there exist one and only one minimal full boundary set $\mathscr{J}$. This analysis excludes the extreme case where $\mathscr{M}$ covers the entire Euclidean space. Furthermore, it is clear that any full boundary necessarily contains the minimal full boundary set.

Figure 1 shows three different cases where set $\mathscr{J}$ is a minimal full boundary to set $\mathscr{M}$; Fig. 2 shows the same three cases with nominal full boundary sets; Fig. 3 shows cases where set $\mathscr{M}$ is empty for given boundary sets.

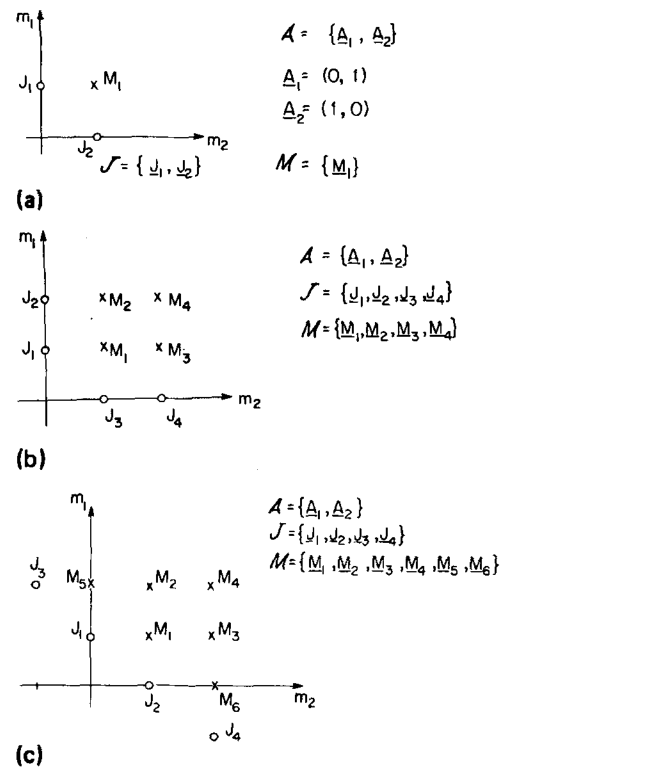

FIG. 1. The Euclidean space considered is two-dimensional. The set of displacement vectors $\mathscr{A}$ contains two elements $\mathbf{A}_1 = (0,1)$ and $\mathbf{A}_2 = (1,0)$. *In case* (*a*) set $\mathscr{M}$ has only one element $\mathbf{M} = (1,1)$ and its minimal full boundary $\mathscr{J}$ contains two elements $\mathbf{J}_1 = (0,1)$ and $\mathbf{J}_2 = (1,0)$. *In case* (*b*) set $\mathscr{M}$ has four elements $\mathbf{M}_1 = (1,1)$, $\mathbf{M}_2 = (1,2)$, $\mathbf{M}_3 = (2,1)$, $\mathbf{M}_4 = (2,2)$ and its minimal full boundary $\mathscr{J}$ contains four elements $\mathbf{J}_1 = (0,1)$, $\mathbf{J}_2 = (0,2)$, $\mathbf{J}_3 = (1,0)$, $\mathbf{J}_4 = (2,0)$. *Finally case* (*c*) corresponds to $\mathscr{M}$ having the four elements of case (b) and two additional ones, $\mathbf{M}_5 = (0,2)$, $\mathbf{M}_6 = (2,0)$, while the minimal full boundary has in addition to those of case (a) $\mathbf{J}_3 = (-1,2)$ and $\mathbf{J}_4 = (2,-1)$.

B. Unrestricted discrete paths in an n-dimensional Euclidean space

In this section we will refer to the *same sets* $\mathscr{M}$, $\mathscr{J}$ and $\mathscr{A}$ as those introduced in Sec. IIA. By definition we know that, for every element $\mathbf{M}$ of $\mathscr{M}$, it is possible to find at least one restricted path connecting $\mathbf{M}$ to at least one element of $\mathscr{J}$. Here we will be considering all possible paths that connect in an *unrestricted* way point $\mathbf{J}$ to point $\mathbf{M}$, in the sense that, intermediate points along the path are *allowed* to be points belonging to $\mathscr{J}$. In other words, restriction (2.6) is deleted, everything else remaining the same as before. Thus the set of unrestricted discrete paths include the set of restricted paths.

If $q_{\max}(\omega)$ is the number of distinct (unrestricted) paths connecting $\mathbf{J}$ to $\mathbf{M}$ into ω discrete steps, then, again, there is a one-to-one correspondence between the distinct paths (ωq) and the distinct sets $\Delta_{\omega q}$. Whenever a path connecting $\mathbf{J}$ to $\mathbf{M}$ into ω steps belonging to $\mathscr{A}$ is not possible, then $q_{\max}(\omega) = 0$ and set $\Delta_{\omega q}$ is an empty set. Thus only certain values of ω may lead to possible unrestricted paths. The set of possible values of ω leading to possible paths will be called $\Omega(\mathbf{M})$. The set will never be empty unless $\mathscr{M}$, is empty.

Let $\mathscr{D}(\omega)$ be the grand set whose elements are the sets $\Delta_{\omega q}$ corresponding to a *given* value of ω, i.e.,

$$\mathscr{D}(\omega) = \{\Delta_{\omega q}; q = 1,\ldots,q_{\max}(\omega)\}, \tag{2.9}$$

and $\overline{\mathscr{D}}$ the grand set whose elements are all sets $\Delta_{\omega q}$;

$$\overline{\mathscr{D}} = \{\Delta_{\omega q}; \omega\in\Omega; q = 1,2,\ldots,q_{\max}(\omega)\} \tag{2.10a}$$

$$= \bigcup_{\omega\in\Omega} \mathscr{D}(\omega). \tag{2.10b}$$

Since there is a one-to-one correspondence between distinct paths and distinct sets Δ, the set of distinct paths into ω steps is isomorphic to $\overline{\mathscr{D}}(\omega)$ and the set of *all* distinct paths regardless of the number of steps is isomorphic to $\mathscr{D}$. Furthermore, we denote by $\mathscr{D}^{\alpha}_{\mathbf{A}_k}(\omega)$ the grand set of ordered sets $\Delta_{\omega q}$ with a given value of ω and whose αth element is restricted to be $\mathbf{A}_k$:

$$\mathscr{D}^{\alpha}_{\mathbf{A}_k}(\omega) = \{\Delta_{\omega q}; \boldsymbol{\delta}_\alpha = \mathbf{A}_k; q = 1,\ldots,q_{\max}(\omega)\}. \tag{2.11}$$

Finally, let $\mathscr{A}''(\omega)$ be the subset of $\mathscr{A}$ containing all displacement vectors $\mathbf{A}_i$ not entering any path connecting $\mathbf{J}$ to $\mathbf{M}$ into ω steps, and $\mathscr{A}'(\omega)$ its complement. Then

$$\mathscr{A} = \mathscr{A}'(\omega)\cup\mathscr{A}''(\omega) \text{ and } \mathscr{A}'(\omega)\cap\mathscr{A}''(\omega) = \emptyset. \tag{2.12}$$

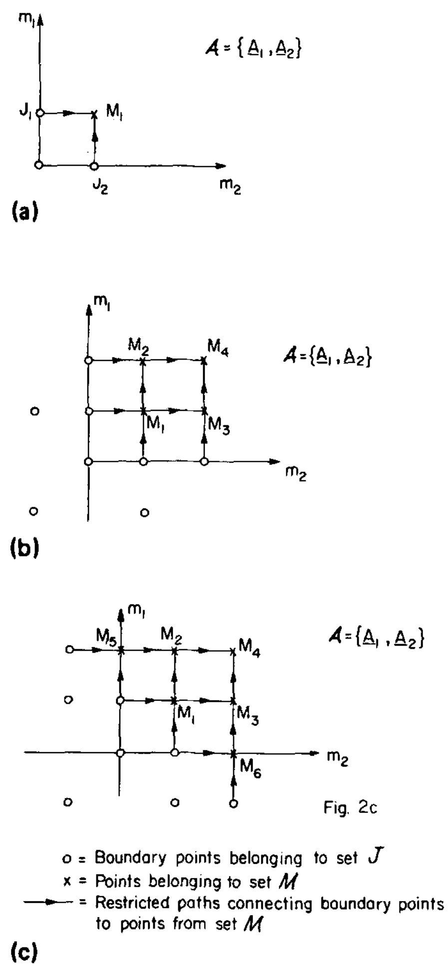

FIG. 2. The three cases represented in Fig. 1. are reproduced here with the same sets $\mathscr{A}$ and $\mathscr{M}$ but with nonminimal full boundaries. Here it is to be noted that no path, leaving any additional boundary point, may reach a point $\mathbf{M}$ of set $\mathscr{M}$ without having at least on of its intermediate points belonging to set $\mathscr{J}$. The only paths represented here are the *restricted* paths.

Similarly, let $\mathscr{A}''$ be the subset of $\mathscr{A}$ containing all displacement vectors $\mathbf{A}_i$ not entering any path connecting $\mathbf{J}$ to $\mathbf{M}$ whatsoever, and $\mathscr{A}'$ its complement. Then again

$$\mathscr{A} = \mathscr{A}' \cup \mathscr{A}'' \text{ and } \mathscr{A}' \cap \mathscr{A}'' = \emptyset. \quad (2.13)$$

So far we only considered the case where point $\mathbf{M}$ is distinct from $\mathbf{J}$. The case $\mathbf{M} = \mathbf{J}$ can be added to our previous discussion by saying that there exists a path connecting $\mathbf{J}$ to $\mathbf{M}$ which is the zero path, for which we set $\omega = 0$ and $q_{max}(0) = 1$.

C. Combinatorics functions

With displacement vectors $\{\mathbf{A}_1, \mathbf{A}_2, ..., \mathbf{A}_N\}$ elements of set $\mathscr{A}$, we associate N functions conveniently denoted by $f_{A_1}, ..., f_{AN}$. With the zero displacement vector $\mathbf{A}_0 = 0$ one associates the function $f_{A_0} = 1$. Furthermore, with a possible path (ωq) connecting $\mathbf{J}$ to $\mathbf{M}$, we associate the functional

$$F_\omega^q(J;M) = \prod_{i=0}^{\omega} w(S_i) f_{\delta_i}(S_i), \ \omega \in \Omega \ q = 1, ..., q_{\max}(\omega), \quad (2.14a)$$

where $\boldsymbol{\delta}_0 = \mathbf{A}_0$ and $\boldsymbol{\delta}_i$, $i = 1, ..., \omega$ are the elements of the ordered set $\Delta_{\omega q}$ and the $\mathbf{S}_i$ are related to the $\mathbf{S}_i$ according to Eqs. (2.4) and (2.5) and not restricted by Eq. (2.6). $w(\mathbf{S}_i)$ is a weight coefficient that can take the values 0 or 1;

$$w(\mathbf{S}_i) = 0 \text{ for } \mathbf{S}_i \in \mathscr{J} \text{ and } i \neq 0,$$

$$w(\mathbf{S}_i) = 1 \text{ otherwise.} \quad (2.14b)$$

The weight coefficient w has the property of setting $F_q^\omega = 0$ for paths connecting $\mathbf{J}$ to $\mathbf{M}$ having at least one of their intermediate points belonging to set $\mathscr{J}$. In other words,

$$F_\omega^q(\mathbf{J};\mathbf{M}) = \prod_{i=0}^{\omega} f_{\delta_i}; \ \mathbf{S}_i \notin \mathscr{J} \text{ for } i \neq 0 \quad (2.14c)$$

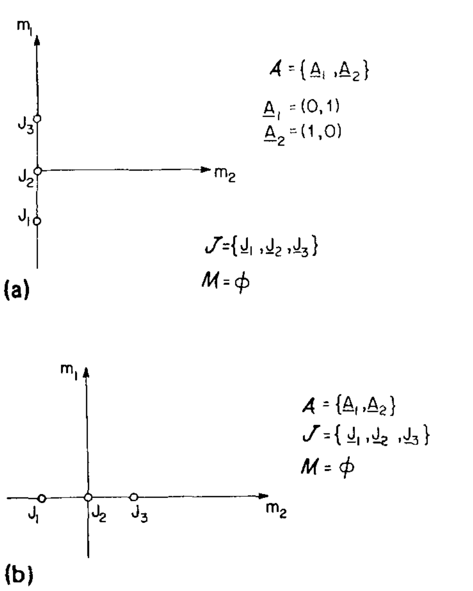

FIG. 3. Here again the Euclidean space space is two-dimensional and the set $\mathscr{A}$ is the same as the one considered in Figs. 1 and 2. Cases (a) and (b) correspond to boundary set $\mathscr{J}$ leading to an empty set $\mathscr{M}$.

only for those paths q restricted by Eq. (2.6). When no path into ω teps belonging to $\mathscr{A}$ is possible, then $\omega \notin \Omega$ ($\mathbf{M}$) and $q_{\max}(\omega) = 0$, and, in this case, we define

$$F_\omega^q(\mathbf{J};\mathbf{M}) = 0, \ \omega \notin \Omega\,(\mathbf{M}). \quad (2.14d)$$

Since $q_{max}(\omega) = 0$ implies that $\omega \notin \Omega$ and that $F_\omega^q(\mathbf{J};\mathbf{M})$ is zero, it is convenient to define

$$F_\omega^0(\mathbf{J};\mathbf{M}) = 0. \quad (2.14e)$$

With all these definitions, when $\mathbf{J} = \mathbf{M}$, $\mathbf{J}$ can be connected to $\mathbf{M}$ by the zero path. In this case $\omega = 0$, and, consequently, $q_{\max}(0) = 1$ only for $\mathbf{J} = \mathbf{M}$. For this special case

$$F_0^1(\mathbf{J};\mathbf{J}) = \prod_{i=0}^{\omega=0} w(\mathbf{S}_i) f_{\delta_i}(\mathbf{S}_i) = 1. \quad (2.14f)$$

By summing the functionals $F_\omega^q(\mathbf{J};\mathbf{M})$ over all distinct paths connecting $\mathbf{J}$ to $\mathbf{M}$ into ω steps, we obtain the combinatorics function of the first kind,

$$C_1(\mathbf{J};\mathbf{M};\omega) = \sum_{q=0}^{q_{\max}(\omega)} F_\omega^q(\mathbf{J};\mathbf{M}). \quad (2.15)$$

On the other hand, by summing the functions, F_ω^q, over all district paths we obtain the combinatorics functions of the second kind,

$$C_2(\mathbf{J};\mathbf{M}) = \sum_\omega \sum_{q=0}^{q_{\max}(\omega)} F_\omega^q(\mathbf{J};\mathbf{M}). \quad (2.16)$$

From Eq. (2.14) defining $F_\omega^q(\mathbf{J};\mathbf{M})$, it is seen that the values of $\omega \notin \Omega$ will certainly give a zero contribution to the summation in Eq. (2.16) Consequently, Eq. (2.16) can also be written as

$$C_2(\mathbf{J};\mathbf{M}) = \sum C_1(\mathbf{J};\mathbf{M};\omega). \quad (2.17)$$

In particular, according to Eqs. (2.14), (2.15), and (2.17) one has

$$C_2(\mathbf{J};\mathbf{J}) = C_1(\mathbf{J};\mathbf{J};0) = f_0(\mathbf{J}) = 1. \quad (2.18)$$

and

$$C_2(\mathbf{J};\mathbf{M}) = 0 = C_1(\mathbf{J};\mathbf{M};\omega), \ \mathbf{M} \notin \mathscr{M}, \quad (2.19a)$$

$$C_1(\mathbf{J};\mathbf{M};\omega) = 0, \ \omega \notin \Omega\,(\mathbf{M}). \quad (2.19b)$$

D. Fundamental theorems

We will now prove two theorems very similar to Theorems 1 and 2 of Ref. 4 on linear one-dimensional recursion relations with a limited type of boundary points. Although there is a striking similarity between what is done here and in Ref. 4, completeness and mathematical rigor demand a separate and distinct development. The language of Ref. 4 uses the words "partition", "partitioning subintervals", "Special Combinatorics Functions" and "Constrained Combinatorics Functions." Here, these objects are replaced by "restricted or unrestricted path", "discrete displacement vectors or steps", and, just "Combinatorics Functions", respectively. All the objects of Refs. 4, 5 and 6 are recovered from our generalized comcepts when the underlying Euclidean space is simply one-dimensional.

In all subsequent developments, $\mathscr{M}$ is the set of all points $\mathbf{M}$ such that all possible paths reaching point $\mathbf{M}$ by successive discrete steps belonging to $\mathscr{A}$ must necessarily contain one and only one boundary point belonging to $\mathscr{J}$. Thus, for every point $\mathbf{M}\in\mathscr{M}$, there exists at least one *restricted path* that links $\mathbf{M}$ to at least one point $\mathbf{J}\in\mathscr{J}$, such that all intermediate steps belong to $\mathscr{A}$ and none of the intermediate points along the path are allowed to be points belonging to $\mathscr{J}$. When such a relationship exists between sets $\mathscr{J}$, $\mathscr{M}$, and $\mathscr{A}$, we focus our attention on two points $\mathbf{J}$ and $\mathbf{M}$ belonging to sets $\mathscr{J}$ and $\mathscr{M}$, respectively, and, the, consider all possible *unrestricted paths*, labeled (ωq), linking $\mathbf{J}$ to $\mathbf{M}$. These unrestricted paths have all their intermediate steps belonging to $\mathscr{A}$, but intermediate points along any path are allowed to be elements of $\mathscr{J}$. Clearly, for two such points $\mathbf{J}$ and $\mathbf{M}$, the set of all *unrestricted paths* includes the set of *restricted paths*.

To simplify the proof of the two theorems on Combinatorics Functions, as in Ref. 4, five lemmas will be needed.

Lemma 1: For every $\mathbf{A}_k\in\mathscr{A}'(\omega)$, there exists at least one unrestricted path connecting $\mathbf{J}$ to $\mathbf{M}$ in ω steps, having its αth step equal to $\mathbf{A}_k$.

Proof: Given a positive integer $\alpha<\omega$ and a displacement vector $\mathbf{A}_k\in\mathscr{A}'(\omega)$, we need to prove the existence of an unrestricted path (ωq) connecting $\mathbf{J}$ to $\mathbf{M}$ in ω steps $(\boldsymbol{\delta}_1,\boldsymbol{\delta}_2,\ldots,\boldsymbol{\delta}_\alpha,\ldots\boldsymbol{\delta}_\omega)$, with $\boldsymbol{\delta}_\alpha=\mathbf{A}_k$. Since $\mathbf{A}_k\in\mathscr{A}'(\omega)$, then by construction of $\mathscr{A}'(\omega)$, there exists at least one unrestricted path $(\omega q')$ connecting $\mathbf{J}$ to $\mathbf{M}$, which includes $\mathbf{A}_k$ as one of its steps. Let this step be $\boldsymbol{\delta}'_i=\mathbf{A}_k$. If $i=\alpha$, then $q=q'$ and the lemma is proved. If $i\neq\alpha$, then the exchange of the two steps $\boldsymbol{\delta}'_i$ and $\boldsymbol{\delta}'_\alpha$ leads to another possible unrestricted path connecting $\mathbf{J}$ to $\mathbf{M}$, since the total number of steps is still ω and the sum of the ω displacement vectors or steps is still $\mathbf{M}$-$\mathbf{J}$. The new path (ωq) obtained by reordering the steps δ' is specified by $\boldsymbol{\delta}_j=\boldsymbol{\delta}'_j$ for $j\neq i$ and $j\neq\alpha$, $\boldsymbol{\delta}_i=\boldsymbol{\delta}'_\alpha$ and $\boldsymbol{\delta}_\alpha=\boldsymbol{\delta}'_i$. Thus $\boldsymbol{\delta}_\alpha=\mathbf{A}_k$ and the lemma is proved.

Lemma 2: The set of unrestricted paths connecting $\mathbf{J}$ to $\mathbf{M}$ into ω steps can be divided into nonempty disjoint subsets which are in one-to-one correspondence with the elements of $\mathscr{A}'(\omega)$.

Proof: Corresponding to each $\mathbf{A}_k\in\mathscr{A}'(\omega)$ we form the subset of unrestricted paths connecting $\mathbf{J}$ to $\mathbf{M}$, whose αth step is $\mathbf{A}_k$. The elements of the subset corresponding to $\mathbf{A}_k$ are represented by $\Delta_{\omega q}\in\mathscr{D}^\alpha_{\mathbf{A}_k}(\omega)$. On the other hand, all unrestricted paths from $\mathbf{J}$ to $\mathbf{M}$ into ω steps are represented by the sets $\Delta_{\omega q}\in\mathscr{D}(\omega)$. What we need to prove is the following:

(i) The subsets $\mathscr{D}^\alpha_{\mathbf{A}_k}(\omega)$ are nonempty and disjoint,

$$\mathscr{D}^\alpha_{\mathbf{A}_k}(\omega)\neq\emptyset \text{ for } \mathbf{A}_k\in 12\mathrm{A}'(\omega), \tag{2.20}$$

and

$$\mathscr{D}^\alpha_{\mathbf{A}_i}(\omega)\cap\mathscr{D}^\alpha_{\mathbf{A}_j}(\omega)=\emptyset \text{ for } i\neq j. \tag{2.21}$$

(ii) $\mathscr{D}(\omega)$ can be divided into the subsets $\mathscr{D}^\alpha_{\mathbf{A}_k}(\omega)$,

$$\mathscr{D}(\omega) \bigcup_{\mathbf{A}_k\in\mathscr{A}'(\omega)} \mathscr{D}^\alpha_{\mathbf{A}_k}(\omega). \tag{2.22}$$

(iii) The correspondence between $\mathscr{D}^\alpha_{\mathbf{A}_k}(\omega)$ and $\mathbf{A}_k\in\mathscr{A}'(\omega)$ is one-to-one.

According to Lemma 1 the subsets $\mathscr{D}^\alpha_{\mathbf{A}_k}(\omega)$ are nonempty for $\mathbf{A}_k\in\mathscr{A}'(\omega)$. Thus Eq. (2.20) is established. Furthermore, if $\Delta_{\omega q}\in\mathscr{D}^\alpha_{\mathbf{A}_i}(\omega)$ then its αth element, $\boldsymbol{\delta}_\alpha$, is $\boldsymbol{\delta}_\alpha=\mathbf{A}_i$. Since the $\mathbf{A}_k$'s are all different, then, for $j\neq i$, $\mathbf{A}_j\neq\mathbf{A}_j$. Consequently $\Delta_{\omega q}\in\mathscr{D}^\alpha_{\mathbf{A}_k}(\omega)$ for any $j\neq i$. Eq. (2.21) is thus established.

Every set $\Delta_{\omega q}$ belonging to $\mathscr{D}(\omega)$ is made up of elements $(\boldsymbol{\delta}_1,\ldots,\boldsymbol{\delta}_\omega)$ belonging to $\mathscr{A}'(\omega)$ by construction of set $\mathscr{A}'(\omega)$. Specifically, the αth element of the ordered set $\Delta_{\omega q}$ is some displacement vector $\mathbf{A}_k\in\mathscr{A}'(\omega)$ and consequently $\Delta_{\omega q}\in\mathscr{D}^\alpha_{\mathbf{A}_k}(\omega)$ corresponds to a path from $\mathbf{J}$ to $\mathbf{M}$ into ω steps and hence belongs to $\mathscr{D}(\omega)$. Eq. (2.22) is thus established.

Finally, since for every $\mathbf{A}_k\in\mathscr{A}'(\omega)$ there exists a nonempty subset $\mathscr{D}^\alpha_{\mathbf{A}_k}(\omega)$, and since two subsets $\mathscr{D}^\alpha_{\mathbf{A}_i}(\omega)$ and $\mathscr{D}^\alpha_{\mathbf{A}_j}(\omega)$, corresponding to two different elements of $\mathscr{A}'(\omega)$, are disjoint, then the correspondence between the subsets $\mathscr{D}^\alpha_{\mathbf{A}_k}(\omega)$ and $\mathbf{A}_k$ of $\mathscr{A}'(\omega)$ is one-to-one.

Lemma 3: There is a one-to-one correspondence between the unrestricted paths from $\mathbf{J}$ to $\mathbf{M}$ into ω steps $(\omega\geqslant 1)$ having their αth step equal to $\mathbf{A}_k$, and the unrestricted paths from $\mathbf{J}$ to $\mathbf{M}-\mathbf{A}_l$ into $(\omega-1)$ steps.

Proof: (i) Case $\omega=1$: An unrestricted path from $\mathbf{J}$ to $\mathbf{M}$ having one step is possible, when $\mathbf{M}-\mathbf{J}=\mathbf{A}_k$ for some $\mathbf{A}_k\in\mathscr{A}$. Since the A's are all different, then there exists only one possible unrestricted path from $\mathbf{J}$ to $\mathbf{M}$ into one path. Furthermore, the path connecting $\mathbf{J}$ to $\mathbf{M}-\mathbf{A}_k$ is the zero path, and thus corresponds to $(\omega-1)=0$ steps which can be done in one and only one way, $q_{\max}(0)=1$. Consequently, the one-to-one correspondence is trivially established in this case.

(ii) Case $\omega\geqslant 2$: Consider an unrestricted path into ω steps $(\boldsymbol{\delta}_1,\boldsymbol{\delta}_2,\ldots,\boldsymbol{\delta}_{\alpha-1},\mathbf{A}_k,\boldsymbol{\delta}_{\alpha+1}\ldots,\delta_\omega)$ connecting $\mathbf{J}$ to $\mathbf{M}$ with $\boldsymbol{\delta}_\alpha=\mathbf{A}_k$, then the path represented by

$$(\boldsymbol{\delta}'_1,\ldots,\boldsymbol{\delta}'_{\omega-1})=(\delta_1,\ldots,\delta_{\alpha-1},\delta_{\alpha+1},\ldots,\delta_\omega) \tag{2.23}$$

is an unrestricted path joining $\mathbf{J}$ to $\mathbf{M}-\mathbf{A}_k$ into $(\omega-1)$ steps, since

$$\sum_{i=1}^{\omega-1}\boldsymbol{\delta}_i=\left(\sum_{i=1}^{\omega}\boldsymbol{\delta}_i\right)-\boldsymbol{\delta}_\alpha=(\mathbf{M}-\mathbf{J})-\mathbf{A}_k=(\mathbf{M}-\mathbf{A}_k)-\mathbf{J}. \tag{2.24}$$

Furthermore, two distinct paths, (ωq_1) and (ωq_2), connecting $\mathbf{J}$ to $\mathbf{M}$ into ω steps and having $\boldsymbol{\delta}_\alpha=\mathbf{A}_k$ must differ by at least one step, say $\boldsymbol{\delta}^1_l\neq\boldsymbol{\delta}^2_l$, for some $l\neq\alpha$. Thus, they will lead to two distinct paths, $(\omega-1,q'_1)$ and $(\omega-1,q'_2)$, connecting $\mathbf{J}$ to $(\mathbf{M}-\mathbf{A}_k)$ into $(\omega-1)$ steps, according to the correspondence established by Eq. (2.23). Conversely, consider a path from $\mathbf{J}$ to $\mathbf{M}-\mathbf{A}_k$ into $(\omega-1)$ steps represented by $(\boldsymbol{\delta}'_1,\boldsymbol{\delta}'_2,\ldots,\boldsymbol{\delta}'_{\omega-1})$. Then $\mathbf{M}$ belongs to set $\mathscr{M}$ and the set

$$(\boldsymbol{\delta}_1,\ldots,\boldsymbol{\delta}_\omega)=(\boldsymbol{\delta}'_1,\ldots,\boldsymbol{\delta}'_{\alpha-1},\mathbf{A}_k,\boldsymbol{\delta}'_\alpha,\ldots,\boldsymbol{\delta}'_\omega) \tag{2.25}$$

represents a path from $\mathbf{J}$ to $\mathbf{M}$ into ω steps since

$$\sum_{i=1}^{\omega}\boldsymbol{\delta}_i=\left(\sum_{i=1}^{\omega-1}\boldsymbol{\delta}'_i\right)+\mathbf{A}_k=(\mathbf{M}-\mathbf{A}_k)-\mathbf{J}+\mathbf{A}_k$$
$$=\mathbf{M}-\mathbf{J}. \tag{2.26}$$

Furthermore, it is clear, according to Eq. (2.25), that two distinct unrestricted paths from $\mathbf{J}$ to $\mathbf{M}-\mathbf{A}_k$ into $(\omega-1)$ steps lead to two distinct unrestricted paths from $\mathbf{J}$ to $\mathbf{M}$ into ω steps.

Thus, the correspondence established in Eq. (2.23) is one-to-one.

Lemma 4: Two points, $\mathbf{J}\in\mathbf{J}$ and $\mathbf{M}-\mathbf{A}_k\in\mathscr{M}$, can be connected by unrestricted paths into $(\omega-1)$ steps, $\omega\geqslant 1$, if and only if $\mathbf{J}$ can be connected to $\mathbf{M}$ by unrestricted paths into ω steps and $\mathbf{A}_k\in\mathscr{A}'(\omega)$.

Proof: The above lemma can be restated as follows:

$$(\omega-1)\in\Omega\,(\mathbf{M}-\mathbf{A}_k)\rightleftarrows\omega\in\Omega\,(\mathbf{M}) \text{ and } \mathbf{A}_k\in\mathscr{A}'(\omega). \quad (2.27)$$

(i) $\omega\in\Omega\,(\mathbf{M})$ and $\mathbf{A}_k\in\mathscr{A}'(\omega)$: Then by construction of $\mathscr{A}'(\omega)$, there exists at least one unrestricted path from **J** to **M** into ω steps, which includes $\mathbf{A}_k$ as one of its steps. The existence of a corresponding path from **J** to $\mathbf{M}-\mathbf{A}_k$ into $(\omega-1)$ steps is then guaranteed by Lemma 3. Hence $(\omega-1)\in\Omega(\mathbf{M}-\mathbf{A}_k)$.

(ii) $(\omega-1)\in\Omega(\mathbf{M}\mathbf{A}_k)$: In this case $(\mathbf{M}-\mathbf{A}_k)$ can be linked to **J** into $(\omega-1)$ steps. Then, by Lemma 3, there exist corresponding paths from **J** to **M** in ω steps, having one of their steps equal to $\mathbf{A}_k$. This means $\omega\in\Omega\,(\mathbf{M})$ and $\mathbf{A}_k\in\mathscr{A}(\omega)$.

Lemma 5: $\mathbf{M}\in\mathscr{M}$ if and only if $\mathbf{M}\text{-}\mathbf{A}_i\notin\mathscr{M}$ for all $\mathbf{A}_i\in\mathscr{A}$. Conversely, $\mathbf{M}\in\mathscr{M}$ if and only if $\mathbf{M}\text{-}\mathbf{A}_i\in\mathscr{M}$ for all $\mathbf{A}_i\in\mathscr{A}$.

Proof: The proofs of the two parts of this lemma are similar. Here, we will only prove the first part since the proof of the second part can be done following similar steps.

(i) $\mathbf{M}\notin\mathscr{M}$: In this case "backward"steps belonging to $\mathscr{A}$ from **M** can only reach points $\mathbf{M}-\mathbf{A}_i$. None of these latter points can be a point belonging to $\mathscr{F}$ since we would have had a restricted path connecting **M** to one of the boundary points (and this is not possible since $\mathbf{M}\notin\mathscr{M}$). Let us assume that one of the points $\mathbf{M}-\mathbf{A}_i$ does belong to set $\mathscr{M}$ for some $i=k$. This would mean that there exists at least one restricted path joining $\mathbf{M}-\mathbf{A}_k$ to at least one of the boundary points, say $\mathbf{J}_l$, and, therefore, there would exist a restricted path joining $\mathbf{J}_l$ to **M** whose last step is $\mathbf{A}_k$, i.e., $\mathbf{M}\in\mathscr{M}$. This contradicts our hypothesis and we conclude that $\mathbf{M}-\mathbf{A}_k\notin\mathscr{M}$.

(ii) $\mathbf{M}-\mathbf{A}_i\notin\mathscr{M}$ for all $\mathbf{A}_i\in\mathscr{A}$: Leaving one of the points, say $\mathbf{M}-\mathbf{A}_k$, point **M** can be reached by a "forward" step $\mathbf{A}_k$. Therefore, restricted paths are not possible connecting any boundary point to point **M** and containing as intermediate (before last) point $\mathbf{M}-\mathbf{A}_k$. Since every possible path reaching point **M** should necessarily contain one of the points $\mathbf{M}-\mathbf{A}_i$, then no restricted paths are possible connecting any boundary point to **M**, and, consequently $\mathbf{M}\notin\mathscr{M}$.

Theorem 2: Given a set $\mathscr{F}$, which is a full boundary of a set $\mathscr{M}$ with respect to a set $\mathscr{A}$ of displacement vectors, and given two points $\mathbf{J}\in\mathscr{F}$ and $\mathbf{M}\in\mathscr{F}$, then, for $\omega\geqslant 1$

$$C_1(\mathbf{J};\mathbf{M};\omega)=\sum_{\mathbf{A}_k\in\mathscr{A}} f_{A_k}(\mathbf{M})C_1(\mathbf{J};\mathbf{M}-\mathbf{A}_k;\omega-1). \quad (2.28)$$

Proof: Eq. (2.28) is trivially satisfied for $\mathbf{M}\notin\mathscr{M}$. Indeed, according to Lemma 5, $\mathbf{M}-\mathbf{A}_k\notin\mathscr{M}$ for all $\mathbf{A}_k\in\mathscr{A}$, and, by construction of the combinatorics functions, namely Eq. (2.19a), both $C_1(\mathbf{J};\mathbf{M};\omega)$ and $C_1(\mathbf{J};\mathbf{M}\text{-}\mathbf{A}_k;\omega-1)$ for any $\mathbf{A}_k\in\mathscr{A}$ vanish. We are left with the less trivial situation $\mathbf{M}\in\mathscr{M}$.

By construction of the combinatorics functions, C_1 corresponds to all possible unrestricted paths connecting **J** to **M**. According to Eq. (2.12), the summation over $\mathbf{A}_k$ in Eq. (2.28) can be separated into two parts:

$$\sum_{\mathbf{A}_k\in\mathscr{A}}=\sum_{\mathbf{A}_k\in\mathscr{A}'(\omega)}+\sum_{\mathbf{A}_k\in\mathscr{A}''(\omega)}. \quad (2.29)$$

By Lemma 4, Eq. (2.27), if $\mathbf{A}_k\in\mathscr{A}'(\omega)$, then $(\omega-1)\in\Omega\,(\mathbf{M}-\mathbf{A}_k)$. Thus by constuction of C_1, one has

$$C_1(\mathbf{J};\mathbf{M}-\mathbf{A}_k;\omega-1)=0 \text{ for } \mathbf{A}_k\in\mathscr{A}''(\omega).$$

Consequently,

$$\sum_{\mathbf{A}_k\in\mathscr{A}''(\omega)} f_{\mathbf{A}_k}(\mathbf{M})C_1(\mathbf{J};\mathbf{M}-\mathbf{A}_k;\omega-1)=0. \quad (2.30)$$

In evaluating the sum over the elements of $\mathscr{A}'(\omega)$, it is convenient to treat separately the cases $\omega\notin\Omega\,(\mathbf{M})$ and $\omega\in\Omega\,(\mathbf{M})$:

(i) The case $\omega\notin\Omega\,(\mathbf{M})$: In this case no path connecting **J** to **M** into ω steps is possible. Thus, by Lemma 4, Eq. (2.27), no path from **J** to $\mathbf{M}-\mathbf{A}_k$ into $(\omega-1)$ steps is possible either, since $(\omega-1)\notin\Omega\,(\mathbf{M}-\mathbf{A}_k)$. Consequently, according to the way the combinatorics functions are defined, $C_1(\mathbf{J};\mathbf{M};\omega)$ and $C_1(\mathbf{J};\mathbf{M}-\mathbf{A}_k;\omega-1)$ are zero for all $\mathbf{A}_k\in\mathscr{A}$. Equation (2.28) is thus trivially satisfied.

(ii) The case $\omega\in\Omega\,(\mathbf{M})$: In this case $\Omega\,(\mathbf{M})\neq\emptyset$ and $\mathbf{M}\in\mathscr{M}$. We will consider the cases $\omega=1$ and $\omega>1$ separately.

(a) $\omega=1$: Then the path from **J** to **M** has only one step, say $\mathbf{A}_t\in\mathscr{A}$. Hence $\mathscr{A}'(\omega)=\{\mathbf{A}_t\}$ has only one element and $\mathbf{M}-\mathbf{A}_t=\mathbf{J}$. By construction

$$C_1(\mathbf{J};\mathbf{M};1)=C_1(\mathbf{J};\mathbf{J}+\mathbf{A}_t;1)=f_{A_t}(\mathbf{M})w(\mathbf{M}),$$

and $w(\mathbf{M})=1$ since $\mathbf{M}\notin\mathscr{F}$. Furthermore, by construction

$$C_1(\mathbf{J};\mathbf{M}-\mathbf{A}_t;0)=C_1(\mathbf{J};\mathbf{J};0)=1.$$

and the theorem is proved.

(b) $\omega\geqslant 2$: For this case we will present the main steps in the derivation in succession, and justify the passage from one stage to the other subsequently. Our starting point is the definition of the combinatorics function of the first kind:

$$C_1(\mathbf{J};\mathbf{M};\omega)=\sum_{q=0}^{q_{\max}(\omega)} F_\omega^q(\mathbf{J};\mathbf{M}) \quad (2.31\text{a})$$

$$=\sum_{\Delta_{\omega q}\in\mathscr{D}(\omega;\mathbf{M})} F_\omega^q(\mathbf{J};\mathbf{M}) \quad (2.31\text{b})$$

$$=\sum_{\mathbf{A}_k\in\mathscr{A}'(\omega)}\ \sum_{\Delta_{\omega q}\in\mathscr{D}''_{\mathbf{A}_k}(\omega;\mathbf{M})} F_\omega^q(\mathbf{J};\mathbf{M}) \quad (2.31\text{c})$$

$$=\Bigg(\sum_{\mathbf{A}_k\in\mathscr{A}'(\omega)} w(\mathbf{M})f_{A_k}(\mathbf{M}) \times \sum_{\Delta_{\omega q}\in\mathscr{D}''_{\mathbf{A}_k}(\omega;\mathbf{M})}\ \prod_{i=0}^{\omega-1} w(\mathbf{S}_i)f_{\delta_i}(\mathbf{S}_i)\Bigg) \quad (2.31\text{d})$$

$$=\sum_{\mathbf{A}_k\in\mathscr{A}'(\omega)}\Bigg(f_{A_k}(\mathbf{M}) \times \sum_{\Delta_{\omega-1,q}\in\mathscr{D}(\omega-1;\mathbf{M}-\mathbf{A}_k)}\ \prod_{i=0}^{\omega-1} w(\mathbf{S}_i)f_{\delta_i}(\mathbf{S}_i)\Bigg) \quad (2.31\text{e})$$

$$=\sum_{\mathbf{A}_k\in\mathscr{A}'(\omega)}\Bigg(f_{A_k}(\mathbf{M}) \times \sum_{\Delta_{\omega-1,q}\in\mathscr{D}(\omega-1;\mathbf{M}-\mathbf{A}_k)} F_{\omega-1}^q(\mathbf{J};\mathbf{M}\text{-}\mathbf{A}_k)\Bigg) \quad (2.31\text{f})$$

$$=\sum_{\mathbf{A}_k\in\mathscr{A}'(\omega)}\Bigg(f_{A_k}(\mathbf{M})\sum_{q=1}^{q_{\max}(\omega-1)} F_{\omega-1}^q(\mathbf{J};\mathbf{M}-\mathbf{A}_k)\Bigg) \quad (2.31\text{g})$$

$$=\sum_{\mathbf{A}_k\in\mathscr{A}'(\omega)} f_{\mathbf{A}_k}(\mathbf{M})C_1(\mathbf{J};\mathbf{M}-\mathbf{A}_k;\omega-1). \quad (2.32)$$

An unrestricted path (ωq) from **J** to **M** into ω steps exists and is represented by the ordered set $\Delta_{\omega q}$, whose elements are the steps in the path ordered from **J** to **M**. Hence the summation over the index q in Eq. (2.31a) can be equivlently performed over the sets $\Delta_{\omega q}$ belonging to the grand set $\mathscr{D}(\omega;\mathbf{M})$, as in Eq. (2.31b). Here we added the argument **M** in referring to the grand set $\mathscr{D}(\omega)$ to make explicit the end point **M** of the path.

The passage from Eq. (2.31b) to Eq. (2.31c) is allowed by Lemma 2 as expressed by Eqs. (2.20), (2.21), and (2.22), with $\alpha = \omega$. Again, we make explicit the relation of $\mathscr{D}^{\omega}_{\mathbf{A}}(\omega)$ to the end point **M**, by writing $\mathscr{D}^{\omega}_{\mathbf{A}_k}(\omega;\mathbf{M})$. $\mathscr{D}^{\omega}_{\mathbf{A}_k}(\omega;\mathbf{M})$ is a subset of the grand set $\mathscr{D}(\omega;\mathbf{M})$ whose elements are the ordered set $\Delta_{\omega q}$. $\mathscr{D}^{\omega}_{\mathbf{A}_k}(\omega;\mathbf{M})$ contains all those $\Delta_{\omega q}$ having their last element $\boldsymbol{\delta}_{\omega} = \mathbf{A}_k$. Since paths are unrestricted and the point $\mathbf{M} - \mathbf{A}_k$ may very well belong to $\mathscr{F}$, despite the fact that $\mathbf{M}\notin\mathscr{F}$, then the displacement $\boldsymbol{\delta}_{\omega} = \mathbf{A}_k$ is unrestricted and is an element of $\mathscr{A}'(\omega)$. This completes the equivalence between Eqs. (2.31b) and (2.31c).

Equation (2.31d) is obtained by using the definition of the functional $\mathbf{F}^q_{\omega}$ as given by Eqs. (2.14) and remembering that we are dealing with the case $\omega\in\Omega(\mathbf{M})$. Furthermore $w(\mathbf{S}_{\omega})f_{A_k}(\mathbf{S}_{\omega})\equiv w(\mathbf{M})f_{A_k}(\mathbf{M})$ has been taken outside the second summation, since the ωth element $\boldsymbol{\delta}_{\omega}$ of all sets $\Delta_{\omega q}$ entering the summation is $\mathbf{A}_k$, and since $\mathbf{S}_{\omega} = \mathbf{M}$ is the same for all paths.

The passage from Eq. (2.31d) to Eq. (2.31e) is made using Lemma 3, according to which there is a one-to-one correspondence between the unrestricted paths from **J** to **M** into ω steps ending by $\mathbf{A}_k$, and the unrestricted paths from **J** to $\mathbf{M} - \mathbf{A}_k$ into $(\omega - 1)$ steps. This is why we made explicit the fact that the grand set $\mathscr{D}(\omega - 1)$ in Eq. (2.31e) refers to the end point $\mathbf{M} - \mathbf{A}_k$ instead of **M**, thus using the notation $\mathscr{D}(\omega - 1;\mathbf{M} - \mathbf{A}_k)$. Finally, this transition is done by using the assumption that $\mathbf{M}\notin\mathscr{F}$, thus requiring $w(\mathbf{M}) = 1$, as stated in Eq. (2.14b).

Since we are considering the case $\omega\in\Omega(\mathbf{M})$, and since, in Eq. (2.31e), $\mathbf{A}_k\in\mathscr{A}'(\omega)$, then according to Lemma 4, $(\omega - 1)\in\Omega(\mathbf{M} - \mathbf{A}_k)$. Thus, using the definition of $\mathbf{F}^q_{\omega}$ as given by Eqs. (2.14), and noting that $\mathbf{S}_{\omega-1} = \mathbf{M}\text{-}\mathbf{A}_k$ for all terms in the second summation of Eq. (2.31e), we obtain Eq. (2.31f).

The second summation of Eq. (2.31f) runs over all the elements of $\mathscr{D}(\omega - 1;\mathbf{M} - \mathbf{A}_k)$ which is in one-to-one correspondence with all unrestricted paths from **J** to $(\mathbf{M} - \mathbf{A}_k)$ into $(\omega - 1)$ steps. This is explicit in Eq. (2.31g) by letting the path label q run over the whole range of possible values, reaching the maximum value $q_{\max}(\omega - 1)$ that depends on the total number of steps $(\omega - 1)$. Finally, Eq. (2.32) is obtained by using the definition of the combinatorics function of the first kind, Eq. (2.15).

Combining Eqs. (2.30) and (2.32), we find that Eq. (2.28) is satisfied for $\omega\geqslant 2$. This completes the proof of Theorem 2.

Theorem 3: Given a set $\mathscr{F}$, which is a full boundary of a set $\mathscr{M}$ with respect to set of displacement vectors $\mathscr{A}$, and given two points $\mathbf{J}\in\mathscr{F}$ and $\mathbf{M}\notin\mathscr{F}$, then

$$C_2(\mathbf{J};\mathbf{M}) = \sum_{\mathbf{A}_k\in\mathscr{A}} f_{A_k}(\mathbf{M})C_2(\mathbf{J};\mathbf{M} - \mathbf{A}_k). \tag{2.33}$$

Proof: Eq. (2.33) is trivially satisfied for $\mathbf{M}\notin\mathscr{M}$. Indeed, according to Lemma 5, $\mathbf{M} - \mathbf{A}_k\notin\mathscr{M}$ for all $\mathbf{A}_k\in\mathscr{A}$, and, by construction of the combinatorics functions, namely Eq. (2.19a), $C_2(\mathbf{J};\mathbf{M})$ and $C_2(\mathbf{J};\mathbf{M} - \mathbf{A}_k)$ are all zero. The case $\mathbf{M}\in\mathscr{M}$ is not trivial and we will present the main steps in the proof in succession and give their justification afterwards:

$$C_2(\mathbf{J};\mathbf{M}) = \sum_{\omega\in\Omega(\mathbf{M})} C_1(\mathbf{J};\mathbf{M};\omega) \tag{2.34a}$$

$$= \sum_{\omega\in\Omega(\mathbf{M})}\sum_{\mathbf{A}_k\in\mathscr{A}} f_{A_k}(\mathbf{M})C_1(\mathbf{J};\mathbf{M} - \mathbf{A}_k;\omega - 1) \tag{2.34b}$$

$$= \sum_{\mathbf{A}_k\in\mathscr{A}} f_{\mathbf{A}_k}(\mathbf{M}) \sum_{\omega\in\Omega(\mathbf{M})} C_1(\mathbf{J};\mathbf{M} - \mathbf{A}_k;\omega - 1) \tag{2.34c}$$

$$= \sum_{\mathbf{A}_k\in\mathscr{A}} \mathrm{f}_{\mathbf{A}_k}(\mathbf{M}) \sum_{(\omega - 1)\in\Omega(\mathbf{M} - \mathbf{A}_k)} C_1(\mathbf{J};\mathbf{M} - \mathbf{A}_k;\omega - 1) \tag{2.34d}$$

$$= \sum_{\mathbf{A}_k\in\mathscr{A}} \mathrm{f}_{\mathbf{A}_k}(\mathbf{M})\, C_2(\mathbf{J};\mathbf{M} - \mathbf{A}_k). \tag{2.34e}$$

The starting point Eq. (2.34a) comes from the relation between the combinatorics functions of the first and second kind as given by Eq. (2.17).

Since $\mathbf{M}\in\mathscr{M}$, then $\omega\geqslant 1$, and the conditions of Theorem 2 are satisfied. Thus using Eq. (2.28) to replace $C_1(\mathbf{J};\mathbf{M};\omega)$ leads to Eq. (2.34b).

The summations over $\mathbf{A}_k\in\mathscr{A}$ and $\omega\in\Omega(\mathbf{M})$ are independent of each other and can therefore be exchanged. Furthermore, $f_{\mathbf{A}_k}(\mathbf{M})$ is independent of ω and can be taken outside the summation over ω. We thus obtain Eq. (2.34c).

According to Lemma 4, $(\omega - 1)\in\Omega(\mathbf{M} - \mathbf{A}_k)$ implies that $\omega\in\Omega(\mathbf{M})$ for $\mathbf{A}_k\in\mathscr{A}$. Thus

$$\{\omega;(\omega - 1)\in\Omega(\mathbf{M} - \mathbf{A}_k)\}\subset\{\omega;\omega\in\Omega(\mathbf{M})\}, \tag{2.35}$$

and consequently

$$\sum_{\omega\in\Omega(\mathbf{M})} C_1(\mathbf{J};\mathbf{M} - \mathbf{A}_k;\omega - 1$$
$$= \sum_{(\omega - 1)\in\Omega(\mathbf{M} - \mathbf{A}_k)} C_1(\mathbf{J};\mathbf{M} - \mathbf{A}_k;\omega - 1)$$
$$+ \sum_{(\omega - 1)\notin\Omega(\mathbf{M} - \mathbf{A}_k),\omega\in\Omega(\mathbf{M})} C_1(\mathbf{J};\mathbf{M} - \mathbf{A}_k;\omega - 1). \tag{2.36}$$

According to Eq. (2.19b) the summation over $(\omega - 1)\notin\Omega(\mathbf{M} - \mathbf{A}_k)$, $\omega\in\Omega(\mathbf{M})$ in Eq. (2.36), adds up to zero. Hence the second term on the right hand side of Eq. (2.36) drops out and the resulting equation substituted in Eq. (2.34c) leads to Eq. (2.34d).

Finally, by using Eq. (2.17) another time we arrive at Eq. (2.34e). Thus Eq. (2.33) is satisfied. This completes the proof of Theorem 3.

III. LINEAR AND HOMOGENEOUS PARTIAL DIFFERENCE EQUATIONS

A. Notation

The general multidimensional linear and homogeneous PDE compactly written as in Eq. (1.3), can be presented explicitly in the form

$$\sum_{k=0}^{N} \mathrm{f}'_k(\mathbf{M}')\, B(\mathbf{M}' - \mathbf{A}'_k) = 0. \tag{3.1}$$

Equation (1.6) is just a special case of Eq. (3.1), where $N = 2$ and the space associated with the PDE is two-dimensional. Thus $\mathbf{M}'$, in Eq. (1.6), stands for (m_1,m_2) and a displacement vectors $\mathbf{A}'_k$ are given as:
$\mathbf{A}'_0 = (0,0)$, $\mathbf{A}'_1 = (-2,1)$, $\mathbf{A}'_2 = (4,-2)$. The multivariable function B, in general, is required to take on specific initial

values at some set of evaluation points that we refer to as boundary conditions, namely,

$$B(\mathbf{J}_1') = \lambda_1, \ldots, B(\mathbf{J}_l') = \lambda_l, \ldots. \tag{3.2}$$

For Eq. (3.1) to be solved, one has to obtain $B(\mathbf{M}')$ in terms of the initial values, λ_l. It is then necessary to be able to connect the evaluation point $\mathbf{M}'$ to the boundary points $\mathbf{J}_l'$ by successive applications of the PDE, Eq. (3.1). This is clearly possible, if and only if, it is possible by successive "backward" discrete steps specified by the displacement vectors $\mathbf{A}_k'$, to reach the boundary points $\mathbf{J}_l'$ and no other points. In other words, if $\mathscr{J}'$ is the set of boundary points and $\mathscr{A}'$ is the set of displacement vectors as specified by the PDE, Eq. (3.1), the only evaluation points $\mathbf{M}'$, for which B can be computed in terms of the λ 's, must belong to a certain set $\mathscr{R}'$, such that $\mathscr{J}'$ is a full boundary of $\mathscr{R}'$ with respect to $\mathscr{A}'$. This simple analysis gives already the answer to the consistency problem between a PDE and its set of initial conditions or initial values. The result will be recovered in a rigorous way in the forthcoming developments.

If there exists at least one coefficient, say f_i', in Eq. (3.1), which is nonzero in the region specified by $\mathscr{R}'$, then it is convenient to divide Eq. (3.1) by $f_i'(\mathbf{M}')$:

$$B(\mathbf{M}' - \mathbf{A}_i') + \sum_{k \neq i} \frac{f_k'(\mathbf{M}')}{f_i'(\mathbf{M}')} B(\mathbf{M}' - \mathbf{A}_k') = 0. \tag{3.3}$$

By setting $\mathbf{M}' - \mathbf{A}_i = \mathbf{M}$, making a shift in the displacement vectors,

$$\mathbf{A}_k = \mathbf{A}_{k-1}' - \mathbf{A}_i' \text{for } k = 1, \ldots, i \tag{3.4a}$$

$$\mathbf{A}_k = \mathbf{A}_k' \text{-} \mathbf{A}_i' \text{for } k = i+1, \ldots, N, \tag{3.4b}$$

and defining new coefficient functions

$$f_{A_k}(\mathbf{M}) = -f_{k-1}'(\mathbf{M} + \mathbf{A}_i')/f_i'(\mathbf{M} + \mathbf{A}_i') \quad \text{for} \quad k = 1, \ldots, i \tag{3.5a}$$

$$f_{A_k}(\mathbf{M}) = -f_k'(\mathbf{M} + \mathbf{A}_i')/f_i'(\mathbf{M} + \mathbf{A}_i') \quad \text{for} \quad k = i+1, \ldots, N, \tag{3.5b}$$

then, the PDE is conveniently written as

$$B(\mathbf{M}) = \sum_{k=1}^{N} f_{A_k}(\mathbf{M}) B(\mathbf{M} - \mathbf{A}_k), \quad \mathbf{M} \in \mathscr{R}. \tag{3.6}$$

The boundary points remain unchanged, say $\mathbf{J}_l = \mathbf{J}_l'$, so that the initial conditions are

$$B(\mathbf{J}_1) = \lambda_1, \ldots, B(\mathbf{J}_l) = \lambda_l, \cdots. \tag{3.7}$$

The set of boundary points $\mathscr{J}$ is identical to $\mathscr{J}'$ while the domain of definition has slightly shifted and is represented by the set $\mathscr{R}$. Also, one has a discrete set of nonzero displacement vectors $\mathscr{A} = \{\mathbf{A}_1, \mathbf{A}_2, \ldots, \mathbf{A}_N\}$. With each displacement vector $\mathbf{A}_k$ one associates a function $f_{A_k}(\mathbf{M})$ which is precisely the coefficient of $B(\mathbf{M} - \mathbf{A}_k)$ in the PDE, Eq. (3.6).

B. General solution

The problem at hand is to give an explicit expression for $B(\mathbf{M})$, in terms of the arbitrary coefficients $f_{A_k}(\mathbf{M})$ and the arbitrary set of initial values $\{\lambda_l; l = 1, 2, \cdots\}$. If the problem has a solution, the since Eq. (3.6) is linear and homogeneous, one expects to be able to obtain $B(\mathbf{M})$ as a linear combination of the initial values, namely,

$$B(\mathbf{M}) = \sum_l C(l)\lambda_l. \tag{3.8}$$

Thus, a coefficient $C(i)$ in the above expansion must be a particular solution of Eq. (3.6) for the case where all the λ 's vanish except for the parameter λ_i which is fixed to be unity. We therefore give the solution in the form of two theorems.

Theorem 4: The combinatorics function of the second kind $C_2(\mathbf{J}_i;\mathbf{M})$ conditions (δ_{il} is Kronecker's symbol)

$$B(\mathbf{J}_l) = \delta_{il}, \quad l = 1, 2, \ldots, i, \cdots, \tag{3.9}$$

provided that all possible discrete paths connecting $\mathbf{J}_i$ to $\mathbf{M}$ are made of displacement vectors $\mathbf{A}_k$ with the associated coefficient functions being f_{A_k}. $\mathbf{A}_k$ and f_{A_k} are as defined by Eq. (3.6).

Proof: Under the conditions specified by this theorem, Theorem 3 can be applied. In particular, Eq. (2.33) is conveniently written as

$$C_2(\mathbf{J}_i;\mathbf{M}) = \sum_{k=1}^{N} f_{A_k}(\mathbf{M}) C_2(\mathbf{J}_i; \mathbf{M} - \mathbf{A}_k), \quad \mathbf{M} \notin \mathscr{J}. \tag{3.10}$$

Furthermore, according to the definition of the combinatorics functions, namely Eqs, (2.14) and (2.15), one has

$$C_2(\mathbf{J}_i;\mathbf{M}) = \sum_{\omega,q} \prod_{j=0}^{\omega} w(\mathbf{S}_j) f_{\boldsymbol{\delta}_j}(\mathbf{S}_j), \tag{3.11}$$

such that $\boldsymbol{\delta}_j \in \mathscr{A}$, $\boldsymbol{\delta}_0 = 0$, $\mathbf{S}_j - \mathbf{S}_{j-1} = \boldsymbol{\delta}_j$, $\mathbf{S}_0 = \mathbf{J}_i$, and $\mathbf{S}_\omega = \mathbf{M}$ for all possible values of ω. The weight coefficient $w(\mathbf{S}_j)$ can take the value 0 or 1, according to

$$w(\mathbf{S}_j) = 0 \quad \text{for} \quad \mathbf{S}_j \in \mathscr{J} \text{ and } j \neq 0$$
$$w(\mathbf{S}_j) = 1 \quad \text{otherwise}. \tag{3.12}$$

It then follows that, if $\mathbf{M}$ is one of the boundary points, $\mathbf{J}_l$, which is not $\mathbf{J}_i$, one has

$$w(\mathbf{S}_\omega) = w(\mathbf{J}_l) = 0 \quad \forall \omega \text{ and } q, \tag{3.13}$$

thus leading to

$$C_2(\mathbf{J}_i, \mathbf{J}_l) = \quad 0 \quad \text{for } i \neq l. \tag{3.14}$$

On the other hand, if $\mathbf{M} = \mathbf{J}_i$, only the zero path connects $\mathbf{J}_i$ to $\mathbf{M}$, corresponding to only one possible value of ω, $\omega = 0$, and a corresponding value of q, $q_{\max}(\omega) = 1$, or

$$C_2(\mathbf{J}_i;\mathbf{J}_i) = w(\mathbf{S}_0) f_{\boldsymbol{\delta}_0}(\mathbf{S}_0) = 1. \tag{3.15}$$

Equations (3.14) and (3.15) can be conveniently combined into one single formula with the use of Kronecker's symbol:

$$C_2(\mathbf{J}_i;\mathbf{J}_l) = \boldsymbol{\delta}_{il}, \quad \mathbf{J}_i \text{and } \mathbf{J}_l \in \mathscr{J}. \tag{3.16}$$

Thus $C_2(\mathbf{J}_i;\mathbf{M})$ satisfies Eq. (3.6) and the boundary condition (3.9). This completes the proof of Theorem 4.

Theorem 5: The solution of Eq. (3.6) with the boundary conditions of Eq. (3.7) is given by

$$B(\mathbf{M}) = \sum_i \lambda_i C_2(\mathbf{J}_i;\mathbf{M}). \tag{3.17}$$

Proof: Since Eq. (3.6) is a linear equation and $C_2(\mathbf{J}_i;\mathbf{M})$ are particular solutions, then any linear combination of the particular solutions must also be a particular solution. Thus $B(\mathbf{M}) = \sum_i \lambda_i C_2(\mathbf{J}_i;\mathbf{M})$ satisfies Eq. (3.6). Furthermore, if one sets $\mathbf{M}$ to be one of the boundary points, say $\mathbf{J}_l$, then, according to Eq. (3.16),

$$B(\mathbf{J}_l) = \sum_i \lambda_i C_2(\mathbf{J}_i;\mathbf{J}_l) = \sum_i \lambda_i \delta_{il} = \lambda_l. \tag{3.18}$$

Thus (3.17) is a solution of Eq. (3.6) and satisfies the boundary conditions (3.7). This completes the proof of Theorem 5.

Corollary 1: $\mathscr{J}$ being the set of boundary points $\{\mathbf{J}_l; l = 1,2,\cdots\}$, and $\mathscr{M}$ the set of points for which $\mathscr{J}$ is a full boundary set with respect to set $\mathscr{A}$ of displacement vectors, then the PDE, Eq. (3.6), is consistent with the set of initial values, Eq. (3.7), if and only if $\mathscr{R} \subset \mathscr{M}$.

Indeed the way the combinatorics functions have been defined, is that they exist if and only if a restricted path exists connecting at least one boundary point to the point $\mathbf{M}$ at which B has to be evaluated. Otherwise, by hand, we set the combinatorics functions to vanish, as stated in Eq. (2.19a). Thus, it is enough for one point $\mathbf{M} \in \mathscr{R}$ not to belong to $\mathscr{M}$ for not being able to compute $B(\mathbf{M})$ in terms of the λ_i's since, according to Eq. (3.17), the C_2's do not exist and are set to be zero. This shows that the domain of definition, $\mathscr{R}$, of the PDE should necessarily be included within $\mathscr{M}$.

Corollary 2: If $\mathscr{R} \subset \mathscr{M}$ and if J_0 is the minimal full boundary of $\mathscr{M}$, then the only initial values, $\lambda_i = B(\mathbf{J}_i)$, in terms of which the evaluation of $B(\mathbf{M})$ can be performed, correspond to the boundary points $\mathbf{J}_i \in \mathscr{J}_0$.

This follows directly from the definition of the minimal full boundary, and the construction of the combinatorics functions.

IV. CONCLUSION

The combinatorics functions, first constructed by Antippa and Phares,[4] to give the solution of one-dimensional, multiterm, linear, and homogeneous recurrence relations for two special sets of initial values, have been generalized to give the solution of the most general multidimensional, multiterm, linear, and homogeneous partial difference equations with arbitrary initial conditions. In the process of generalizing the concept of combinatorics functions of Ref. 4, a better understanding of the construction of the solution of PDE was attained, leading to a very simple criterion of existence of solutions in terms of the predetermined set of initial values. The main results can be summarized as follows: Given the linear partial difference equation

$$B(\mathbf{M}) = \sum_{k=1}^{N} f_{A_k}(\mathbf{M}) B(\mathbf{M} - \mathbf{A}_k), \quad \mathbf{M} \in \mathscr{R}, \tag{4.1}$$

with the initial value conditions

$$B(\mathbf{J}_l) = \lambda_l, \quad \mathbf{J}_l \in \mathscr{J}, \tag{4.2}$$

where $\mathscr{R}$ is the set specifying the domain of definition of the PDE, and $\mathscr{J}$ the set of boundary points $\mathbf{J}_l$, then,

(i) a solution exists if and only if $\mathscr{R} \subset \mathscr{M}$, where $\mathscr{M}$ is the set having $\mathscr{J}$ as a full boundary with respect to set $\mathscr{A} = \{\mathbf{A}_1, \mathbf{A}_2, \ldots, \mathbf{A}_N\}$.

(ii) The solution, when it exists, is unique, since $\mathscr{M}$ has one and only one minimal full boundary $\mathscr{J}_0$, and $B(\mathbf{M})$ is computed in terms of those λ_l corresponding to $\mathbf{J}_l \in \mathscr{J}_0$.

(iii) The solution is given in terms of the combinatorics functions of the second kind as

TABLE I. Functionals associated with all restricted paths connecting boundary point $\mathbf{J}_2$ to point $\mathbf{M}_4$ of Fig. 1c. $\Omega(\mathbf{M}) = \{\omega = 3\}$ for $\mathbf{J}_2 = (1,0)$

ω	Path	Path label q	$F^q_\omega(\mathbf{J}_2,\mathbf{M}_4)$
3	$\mathbf{J}_2\mathbf{M}_1\mathbf{M}_2\mathbf{M}_4$	1	$f_{A_1}(\mathbf{M}_1) f_{A_1}(\mathbf{M}_2) f_{A_2}(\mathbf{M}_4)$
3	$\mathbf{J}_2\mathbf{M}_1\mathbf{M}_3\mathbf{M}_4$	2	$f_{A_1}(\mathbf{M}_1) f_{A_2}(\mathbf{M}_3) f_{A_1}(\mathbf{M}_4)$
3	$\mathbf{J}_2\mathbf{M}_6\mathbf{M}_3\mathbf{M}_4$	3	$f_{A_2}(\mathbf{M}_6) f_{A_1}(\mathbf{M}_3) f_{A_1}(\mathbf{M}_4)$

$$B(\mathbf{M}) = \sum_l \lambda_l C_2(\mathbf{J}_l;\mathbf{M}). \tag{4.3}$$

The combinatorics functions of the second kind are constructed as follows:

(iv) For every $\mathbf{J}_l \in \mathscr{J}_0$ and $\mathbf{M} \in \mathscr{M}$, one considers all possible *restricted* paths connecting $\mathbf{J}_l$ to $\mathbf{M}$ into steps $\boldsymbol{\delta}_i \in \mathscr{A}$. A given restricted path may be labeled (ωq) where ω refers to the number of steps in a path, and q individualizes the particular path into ω steps.

(v) Corresponding to each (ωq) path with steps $(\boldsymbol{\delta}_1, \boldsymbol{\delta}_2, \ldots, \boldsymbol{\delta}_\omega)$, intermediate points $\mathbf{S}_i$ are generated, given by

$$\mathbf{S}_i = \mathbf{J}_l + \sum_{j=1}^{i} \boldsymbol{\delta}_j, \quad \mathbf{S}_i \notin \mathscr{J}, \quad i = 1, \ldots, \omega. \tag{4.4}$$

(vi) Corresponding to each (ωq) path, construct the functional [here the weight coefficient $w(\mathbf{S}_i)$ is automatically 1, since $\mathbf{S}_i \notin \mathscr{J}$]:

$$F^q_\omega(\mathbf{J}_l;\mathbf{M}) = \sum_{i=1}^{\omega} f_{\delta_i}(\mathbf{S}_i). \tag{4.5}$$

(vii) The combinatorics function of the second kind is then given by the sum over all functions corresponding to all distinct restricted paths connecting $\mathbf{J}_l$ to $\mathbf{M}$:

$$C_2(\mathbf{J}_l;\mathbf{M}) = \sum_\omega \sum_q F^q_\omega(\mathbf{J}_l;\mathbf{M}). \tag{4.6}$$

Generalization of the technique to the inhomogeneous PDE and its applications will be presented elsewhere.[9] Finally, in Table I, we consider the particular case of Fig. 1c, where the set $(\mathbf{M}_4)$ contains only one element, $\omega = 3$, for the boundary point $\mathbf{J}_2 = (0,1)$. Restricted paths are then sequentially labeled and the associated functionals F^q_ω are appropriately given.

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A multidimensional extension of the combinatorics function technique. II. Linear and inhomogeneous partial difference equations

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Recently the solution of multidimensional, linear, and homogeneous recurrence relations, or partial difference equations (PDE), was obtained via a multidimensional extension of the combinatorics function technique, developed by Antippa and Phares. Combinatorics functions of the first and second kind are representations of "restricted" paths connecting two points in an n-dimensional space. These functions are shown to give the solution of the most general linear and inhomogeneous PDE. The consistency of the PDE with the initial value conditions is also discussed. Applications of the method are given elsewhere.

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I. INTRODUCTION

The aim of this paper is to obtain the explicit expression of the solutions of the most general linear and inhomogeneous partial difference equations (PDE). This work is the natural extension of a recent article[1] on the linear and homogeneous PDE, hereafter referred to as paper I. All the notations used here are those of paper I, where the homogeneous PDE was conveniently written as

$$B(\mathbf{M}) = \sum_{k=1}^{N} f_{A_k}(\mathbf{M})\, B(\mathbf{M} - \mathbf{A}_k);\ \mathbf{M}\in\mathscr{R}. \tag{1.1}$$

B is a multivariable function and its argument $\mathbf{M}$ stands for a set of n variables $(m_1, m_2,...,m_n)$. Thus $\mathbf{M}$ can also be viewed as a vector in a n-dimensional space representing the coordinates of a point M. Using a loose language we will refer to $\mathbf{M}$ as either the vector or the point it is associated with. Equation (1.1) expresses the property that for certain points $\mathbf{M}$ of the n-dimensional space, specified by region $\mathscr{R}$, $B(\mathbf{M})$ is related to n terms corresponding to the same function B with shifted arguments, $\mathbf{M} - \mathbf{A}_k$. The N shifts or N displacement vectors form a set we call $\mathscr{A} = \{\mathbf{A}_1,\mathbf{A}_2,...,\mathbf{A}_N\}$. The coefficients multiplying $B(\mathbf{M} - \mathbf{A}_k)$ are assumed to be known and are conveniently labeled by A_k. Coefficients $f_{A_k}(\mathbf{M})$ are not necessarily constant and may very well depend on the evaluation point $\mathbf{M}$. Difference equation (1.1) by itself is insufficient to determine uniquely the value of the function B at any evaluation point $\mathbf{M}$ belonging to region $\mathscr{R}$, unless some set of initial values is specified. These values or boundary conditions are the values of B at some arguments $\mathbf{J}_l$, taken as

$$B(\mathbf{J}_l) = \lambda_l;\quad l = 1,2,.... \tag{1.2}$$

The associated points $\mathbf{J}_l$ in the n-dimensional space, called boundary points, form a set $\mathscr{J} = \{\mathbf{J}_l;\ l = 1,2,...\}$ referred to as the "boundary" set.

Equation (1.1) and its boundary value condition, Eq. (1.2), were first discussed by Antippa and Phares[2,3,4] for the special case where B is a single-variable function and therefore defined on a one-dimensional space ($n = 1$).

Equation (1.1) is not necessarily consistent with the boundary value condition, Eq. (1.2). To obtain the consistency condition, it was esssential to introduce in paper I a set, $\mathscr{M}$, containing all points $\mathbf{M}$ in the n-dimensional space not having the following property:

There exists at least one path reaching point $\mathbf{M}$ by successsive discrete steps belong to $\mathscr{A}$ containing no boundary points belonging to $\mathscr{J}$. When such a relationship exists between two sets $\mathscr{M}$ and $\mathscr{J}$, then $\mathscr{J}$ is called a "full boundary" of $\mathscr{M}$ with respect to $\mathscr{A}$. Also in paper I. it was shown that there exists one and only one set, $\mathscr{J}_0$, called the "minimal full boundary" of $\mathscr{M}$, with respect to $\mathscr{A}$, such that each and every element of $\mathscr{J}_0$ can be connected to at least one element of $\mathscr{M}$, by at least one restricted path. We showed in paper I that Eq. (1.1) is consistent with Eq. (1.2) provided $\mathscr{R}\subset\mathscr{M}$, and that, if this is the case, the solution is unique and depends only on those λ's corresponding to boundary points $\mathbf{J}_l\in\mathscr{J}_0$.

The solution of Eq. (1.1), when it exists, is given in terms of the combinatorics functions of the second kind. For every boundary point $\mathbf{J}_l\in\mathscr{J}_0$ and evaluation point $\mathbf{M}\in\mathscr{M}$, one considers all possible restricted paths connecting $\mathbf{J}_l$ to $\mathbf{M}$ by steps $\boldsymbol{\delta}_i\in\mathscr{A}$. A given path is identified by two labels (ωq). ω refers to the number of steps in a path. Label q is used to distinguish among various paths having the same number of steps ω. Corresponding to each (ωq)-path with steps $(\boldsymbol{\delta}_1,\boldsymbol{\delta}_2,...,\boldsymbol{\delta}_\omega)$, intermediate points $\mathbf{S}_i$ are generated by

$$\mathbf{S}_i = \mathbf{J}_l + \sum_{j=1}^{i} \boldsymbol{\delta}_j;\ i = 1,...,\omega;\ \mathbf{S}_\omega = \mathbf{M}. \tag{1.3}$$

With each (ωq) path, one constructs the functional

$$F^q_\omega(\mathbf{J}_l;\mathbf{M}) = \prod_{i=0}^{\omega} w(\mathbf{S}_i)\, f_{\delta_i}(\mathbf{S}_i), \tag{1.4}$$

where $\boldsymbol{\delta}_0 = \mathbf{A}_0 = 0$ refers to the zero-displacements and $f_{\delta_0}\equiv 1$. On the other hand, $w(\mathbf{S}_i)$ is a weight coefficient that may take the values 0 or 1, according to

$$\begin{aligned} &w(\mathbf{S}_i) = 0 \quad \text{if} \quad \mathbf{S}_i\in\mathscr{J} \text{ and } i\neq 0,\\ &w(\mathbf{S}_i) = 1 \text{ otherwise,} \end{aligned} \tag{1.5}$$

i.e., one sets F^q_ω to vanish automatically whenever a path connecting $\mathbf{J}_l$ to $\mathbf{M}$ contains an intermediate point $\mathbf{S}_i$ belonging to $\mathscr{J}$. In other words, F^q_ω does not vanish for the restricted paths connecting $\mathbf{J}$ to $\mathbf{M}$. Finally, the combinatorics function of the second kind associated with the boundary point $\mathbf{J}_l$ and the evaluation point $\mathbf{M}$ is

$$C_2(\mathbf{J}_l;\mathbf{M}) = \sum_\omega \sum_q F^q_\omega(\mathbf{J}_l;\mathbf{M}) \quad (1.6)$$

and the solution of Eq. (1.1) satisfying the boundary value condition (1.2) is given by[1]

$$B(\mathbf{M}) = \sum_l \lambda_l C_2(\mathbf{J}_l;\mathbf{M}). \quad (1.7)$$

Theorem 3 of paper I states that: Given a set $\mathscr{J}$, which is a full boundary of a set $\mathscr{M}$ with respect to a setof displacement vectors $\mathscr{A}$, and given two points $\mathbf{J}\in\mathscr{J}$ and $\mathbf{M}\notin\mathscr{J}$, then

$$C_2(\mathbf{J};\mathbf{M}) = \sum_{\mathbf{A}_k\in\mathscr{A}} f_{A_k}(\mathbf{M})\, C_2(\mathbf{J};\mathbf{M}-\mathbf{A}_k). \quad (1.8)$$

In this paper we need a slight extension of this theorem.

Theorem 1: Given a set $\mathscr{J}$, which is a full boundary of a set $\mathscr{M}$ with respect to a set of displacement vectors $\mathscr{A}$, and given two points $\mathbf{L}$ and $\mathbf{M}\in\mathscr{M}$, and $\mathbf{L}\neq\mathbf{M}$, then

$$C_2(\mathbf{L};\mathbf{M}) = \sum_{A_k\in\mathscr{A}} f_{A_k}(\mathbf{M})\, C_2(\mathbf{L};\mathbf{M}-\mathbf{A}_k). \quad (1.9)$$

The proof of this theorem follows exactly the same steps as those of the proof of Theorem 3 of paper I. Since it is a long and tedious proof with no new insight to be gained from it, it will not be given here. Nevertheless, Eq. (1.9) will play an essential role in completing the theory developed in paper I to include the solutions of linear and inhomogeneous partial difference equations.

II. LINEAR AND INHOMOGENEOUS PARTIAL DIFFERENCE EQUATIONS

The most general multidimensional, linear and inhomogeneous PDE is obtained by adding to the right-hand side of Eq. (1.1) an arbitrary term that may very well depend on the evaluation point $\mathbf{M}$, say $I(\mathbf{M})$, thus leading to

$$B(\mathbf{M}) = I(\mathbf{M}) + \sum_{k=1}^{N} f_{A_k}(\mathbf{M})\, B(\mathbf{M}-\mathbf{A}_k); \quad \mathbf{M}\in\mathscr{R}. \quad (2.1)$$

To completely specify the PDE, one still has to assume a certain set
of initial values, similar to Eq. (1.2)

$$B(\mathbf{J}_l) = \lambda_l; \quad l = 1,2,...; \quad \mathbf{J}_l\in\mathscr{J}. \quad (2.2)$$

The solution of Eq. (2.1) satisfying the boundary value conditions (2.2) will again be given in terms of combinatorics functions.

In Sec. I, we gave a brief review of the combinatorics functions and the way they are related to the existence of restricted paths connecting a boundary point $\mathbf{J}\in\mathscr{J}_0$ to an evaluation point $\mathbf{M}$. For the combinatorics functions to exist, $\mathbf{M}$ has to belong to $\mathscr{M}$. Nevertheless, in paper I, it was convenient to assign the value zero for the combinatorics functions whenever $M\notin\mathscr{M}$. So that, in the final analysis, the solution of the PDE existed if and only if $\mathscr{R}\subset\mathscr{M}$. We expect the same to hold for the inhomogeneous case.

As anticipated in Sec. I, $C_2(\mathbf{L};\mathbf{M})$, where both $\mathbf{L}$ and $\mathbf{M}\in\mathscr{M}$, will play an essential role in obtaining the solution of the inhomogeneous PDE. Following the same convention as in paper I, we set

$$C_2(\mathbf{L};\mathbf{M}) = 0, \quad (2.3a)$$

whenever no restricted paths connecting $\mathbf{L}$ to $\mathbf{M}$ are possible. Otherwise one can construct the functions

$$F^q_\omega(\mathbf{L};\mathbf{M}) = \prod_{i=0}^{\omega} w(\mathbf{S}_i) f_{\delta_i}(\mathbf{S}_i) \quad (2.3b)$$

for every possible path (ωq) connecting $\mathbf{L}$ to $\mathbf{M}$ by discrete steps $\delta_i\in\mathscr{A}$, such that

$$\boldsymbol{\delta}_i = \mathbf{L} + \sum_{j=0}^{i} \boldsymbol{\delta}_j \quad (2.3c)$$

and

$$w(\mathbf{S}_i) = 0 \quad \text{if} \quad \mathbf{S}_i\in\mathscr{J} \quad \text{and} \quad i\neq 0,$$
$$w(\mathbf{S}_i) = 1, \quad \text{otherwise}. \quad (2.3d)$$

This is exactly the same as before, except that the initial starting point on the paths is $\mathbf{L}\in\mathscr{M}$ instead of being an element of $\mathscr{J}$. In particular, the definition

$$C_2(\mathbf{L};\mathbf{M}) = \sum_{\omega,q} F^q_\omega(\mathbf{L};\mathbf{M}) \quad (2.3e)$$

shows that one has the normalization constraint

$$C_2(\mathbf{L};\mathbf{L}) = 1. \quad (2.3f)$$

A. Particular solution

In the first step we search for the solution of Eq. (2.1) satisfying the initial conditions

$$B(\mathbf{J}_l) = 0; \quad \forall \mathbf{J}_l\in\mathscr{J}. \quad (2.4)$$

This solution is given in a form of a theorem.

Theorem 2: The solution of Eq. (2.4) satisfying the initial conditions (2.4) is

$$B_I(\mathbf{M}) = \sum_{\mathbf{L}_j\in\mathscr{M}} I(\mathbf{L}_j)\, C_2(\mathbf{L}_j\mathbf{M};). \quad (2.5)$$

Proof: We are going to show that

$$I(\mathbf{M}) + \sum_{k=1}^{N} f_{A_k}(\mathbf{M})\, B_I(\mathbf{M}-\mathbf{A}_k) \quad (2.6)$$

is indeed equal to $B_I(\mathbf{M})$. In other words, we are going to prove first that $B_I(\mathbf{M})$ satisfies Eq. (2.1).

According to Eq. (2.5), one has

$$B_I(\mathbf{M}-\mathbf{A}_k) = \sum_{\mathbf{L}_j\in\mathscr{M}} I(\mathbf{L}_j)\, C_2(\mathbf{L}_j;\mathbf{M}-\mathbf{A}_k). \quad (2.7)$$

One then substitutes Eq. (2.7) into Eq. (2.6)

$$I(\mathbf{M}) + \sum_{k=1} f_{A_k}(\mathbf{M}) \sum_{\mathbf{L}_j\in\mathscr{M}} I(\mathbf{L}_j)\, C_2(\mathbf{L}_j;\mathbf{M}-\mathbf{A}_k), \quad (2.8)$$

and exchanges the order of the summations

$$I(\mathbf{M}) + \sum_{\mathbf{L}_j\in\mathscr{M}} I(\mathbf{L}_j) \sum_{k=1}^{N} f_{A_k}(\mathbf{M})\, C_2(\mathbf{L}_j;\mathbf{M}-\mathbf{A}_k). \quad (2.9)$$

According to Theorem 1, one has

$$\sum_{k=1}^{N} f_{A_k}(\mathbf{M})\, C_2(\mathbf{L}_j;\mathbf{M}-\mathbf{A}_k) = C_2(\mathbf{L}_j;\mathbf{M}) \quad \text{for } \mathbf{M}\neq\mathbf{L}_j. \quad (2.10)$$

On the other hand, for $\mathbf{M} = \mathbf{L}_j$,

$$C_2(\mathbf{L}_j;\mathbf{L}_j-\mathbf{A}_k) = 0, \quad \mathbf{A}_k\in\mathscr{A}, \quad (2.11)$$

since no "forward" path is possible connecting $\mathbf{L}_j$ to $\mathbf{L}_j - \mathbf{A}_k$; indeed,

$$(\mathbf{L}_j - \mathbf{A}_k) - \mathbf{L}_j = -\mathbf{A}_k \quad \text{and} \quad -\mathbf{A}_k \notin \mathscr{A}. \tag{2.12}$$

Equations (2.10) and (2.11) can be unified into a single expression using property (2.3f) and Kroneckner's symbol, namely,

$$\sum_{k=1}^{N} f_{A_k}(\mathbf{M})\, C_2(\mathbf{J}_j;\mathbf{M}-\mathbf{A}_k) = C_2(\mathbf{L}_j;\mathbf{M}) - \delta_{\mathbf{L}_j,\mathbf{M}}. \tag{2.13}$$

Combining Eqs. (2.9) and (2.13) one finds

$$I(M) + \sum_{L_j \in \mathscr{M}} I(L_j\,[C_2(L_j;\mathbf{M}) - \delta_{L_j,M}\,] = \sum_{\mathbf{L}_j \in \mathscr{M}} I(\mathbf{L}_j) C_2(\mathbf{L}_j;\mathbf{M}). \tag{2.14}$$

By construction the right-hand side of Eq. (2.14) is $B_I(\mathbf{M})$. Thus $B_I(\mathbf{M})$ satisfies the inhomogeneous PDE Eq. (2.1). Furthermore, $B_I(\mathbf{M})$ vanishes at all boundary points $\mathbf{J}_l$:

$$B_I(\mathbf{J}_l) = \sum_{\mathbf{L}_j \in \mathscr{M}} I(\mathbf{L}_j)\, C_2(\mathbf{L}_j;\mathbf{J}_l) \tag{2.15}$$

and

$$C_2(\mathbf{L}_j;\mathbf{J}_l) = 0 \tag{2.16}$$

since no path is possible going *from* $\mathbf{L}_j$ *to* $\mathbf{J}_l$ by steps belonging to $\mathscr{A}$. Indeed $\mathbf{L}_j \in \mathscr{M}$ and paths may exist connecting $\mathbf{J}_l$ to $\mathbf{L}_j$ by forward steps $\mathbf{A}_k \in \mathscr{A}$; but paths from $\mathbf{L}_j$ to $\mathbf{J}_l$ would then involve steps $-\mathbf{A}_k$, and $-\mathbf{A}_k \notin \mathscr{A}$. This completes the proof of Theorem 2.

B. General solution

The problem at hand is to give an explicit expression of the function $B(\mathbf{M})$ in terms of the arbitrary coefficients $f_{A_k}(\mathbf{M})$ and the arbitary set of parameters $\{\lambda_l; l = 1,2,...\}$, as given by Eq. (2.2), specifying the initial value conditions. Again, the general solution will be given in the form of the theorem.

Theorem 3: The solution of Eq. (2.1) satisfying the arbitrary initial value conditions (2.2) is obtained by adding to the particular solution $B_I(\mathbf{M})$ of Theorem 2, the solution $B_H(\mathbf{M})$ of the associated homogeneous equation, Eq. (1.1), with the same initial values (2.2),

$$B_H(\mathbf{M}) = \sum_l \lambda_l C_2(\mathbf{J}_l;\mathbf{M}). \tag{2.17}$$

Proof: The proof of this theorem is done in two steps. We first show that $B(\mathbf{M}) = B_H(\mathbf{M}) + B_I(\mathbf{M})$ satisfies the PDE, Eq. (2.1), and then that it also satisfies the initial conditions (2.2).

(i) By hypothesis $B_H(\mathbf{M})$ and $B_I(\mathbf{M})$ satisfy the difference equations

$$B_H(\mathbf{M}) = \sum_{k=1}^{N} f_{A_k}(\mathbf{M})\, B_H(\mathbf{M}-\mathbf{A}_k), \tag{2.18}$$

$$B_I(\mathbf{M}) = I(\mathbf{M}) + \sum_{k=1}^{N} f_{A_k}(\mathbf{M})\, B_I(\mathbf{M}-\mathbf{A}_k). \tag{2.19}$$

Adding up Eqs. (2.18) and (2.19) we obtain

$$[B_H(\mathbf{M}) + B_I(\mathbf{M})] = I(\mathbf{M}) + \sum_{k=1}^{N} f_{A_k}(\mathbf{M})\,[B_H(\mathbf{M}-\mathbf{A}_k) + B_I(\mathbf{M}-\mathbf{A}_k)]. \tag{2.20}$$

Consequently, $B_H(\mathbf{M}) + B_I(\mathbf{M})$ is a solution of Eq. (2.1).

(ii) Let $B(\mathbf{M}) = B_H(\mathbf{M}) + B_I(\mathbf{M})$. According to Theorem 5 of paper I, we have

$$B_H(\mathbf{J}_l) = \lambda_l, \tag{2.21}$$

and, by construction,

$$B_I(\mathbf{J}_l) = 0. \tag{2.22}$$

so that

$$B(\mathbf{J}_l) = B_H(\mathbf{J}_l) + B_I(\mathbf{J}_l) = \lambda_l. \tag{2.23}$$

Therefore, $B(\mathbf{M})$, given as

$$B(\mathbf{M}) = \sum_{\mathbf{J} \in \mathscr{J}} \lambda_l C_2(\mathbf{J}_l;\mathbf{M}) + \sum_{\mathbf{L} \in \mathscr{M}} I(\mathbf{L})\, C_2(\mathbf{L};\mathbf{M}), \tag{2.24}$$

is the solution of the linear and inhomogeneous PDE, Eq. (2.1), satisfying the initial value condition (2.2). This completes the proof of Theorem 3.

III. THE CONSISTENCY PROBLEM

If $\mathbf{M}$ does not belong to set $\mathscr{M}$, then no restricted path is possible connecting any boundary point, $\mathbf{J}_l$, to $\mathbf{M}$ by discrete displacements $\mathbf{A}_k \in \mathscr{A}$. Furthermore, it is clear from Lemma 5 of paper I, that if $\mathbf{M} \notin \mathscr{M}$ and $\mathbf{L} \in \mathscr{M}$, then again no restricted path is possible connecting $\mathbf{L}$ to $\mathbf{M}$. In this case, $C_2(\mathbf{J}_l;\mathbf{M})$ and $C_2(\mathbf{L};\mathbf{M})$ are both set to be zero, expressing the nonexistence of restricted paths. Consequently, it follows from Eq. (2.34) that the explicit construction of the solution of the PDE exists for only those evaluation points $\mathbf{M}$ belonging to set $\mathscr{M}$. In other words, the consistency of the PDE, Eq. (2.1), with its initial value conditions, Eq. (2.2), is secured if and only if $\mathscr{R} \subset \mathscr{M}$.

As pointed out earlier, if the solution exists, then $B(\mathbf{M})$ depends solely on those parameters λ_l corresponding to points $\mathbf{J}_l$ belonging to the minimal full boundary $\mathscr{J}_0$.

Finally, applications of the multidimensional combinatorics function technique will be presented in forthcoming papers.

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Schrödinger operators with $L_w^{l/2}(\mathbb{R}^l)$-potentials

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We consider the Schrödinger operators $-\Delta + V$ with V in the weak L^q class, with $q = \frac{l}{2}$ the underlying dimension, which is the borderline for a definition to be possible. We concentrate first on optimal bounds on how large the weak norm of V can be and then on spectral properties on L^p spaces.

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In this paper we consider spectral properties of the Schrödinger operator $-\Delta + V$ acting in $L^p(\mathbb{R}^l)$ spaces. Negative potentials will be our special interest. For correct definition of the operator $-\Delta + V$ we assume some boundness conditions on the negative part of the potential V. Namely, in the L^2-case we need a $-\Delta$-form boundness of V (or $V \in PK$ in our terminology), and for the L^p-case we need a $-\Delta$ boundness (in the L^p sense) of the operator V. The sufficient conditions which guarantee $V \in PK$, $V \in P_p$ were obtained by F. Brownell,[1] W. Faris,[2] and have the form: $V \in L^p(\mathbb{R}^l) + L^\infty(\mathbb{R}^l), p \geqslant l/2$. In some other form these conditions were obtained by F. Stummel[3] (see also M. Schechter[4]). But potentials from $L^p(\mathbb{R}^l), p > l/2$ are not of interest here because $\exp(-t(-\Delta + V))$ will then be a C_0-semigroup in the space $C(\mathbb{R}^l)$ which significantly simplifies the situation.

A more general sufficient condition was mainly proved by R. Strichartz[5] in terms of weak $L^p(\mathbb{R}^l)$ spaces. Evidently, this condition is very close to that we need because our aim is to control the value of a weak $L^{l/2}(\mathbb{R}^l)$ norm of the potential. So the Schrödinger operators with the weak $L^{l/2}(\mathbb{R}^l)$ potential are of particular interest.

The plan of our paper is as follows. The definitions of perturbation classes PK, P_p and the proof of $P_p \subset PK$ are given in Sec. 1. Section 2 is devoted to the computation of the best constants in Strichartz's and some related inequalities which are useful for the investigation of $L_w^p(\mathbb{R}^l)$ potentials. Section 3 is based on the results of Sec. 2 and contains the most general at present sufficient conditions for $V \in PK$, $V \in P_p$. There are are some general results about a semigroup generator in L^p spaces in Sec. 4. In Sec. 5 we investigate the first general problem for the Schrödinger operators with $L_w^{l/2}(\mathbb{R}^l)$-potentials. Notice that all early results fit naturally our L^p theory. There is a proof of the exact L^p-estimates for eigenfunctions and generalized eigenfunctions of the Schrödinger operator in Sec. 6.

1. PERTURBATION CLASSES

Let $L^p \equiv L^p(\mathbb{R}^l)$ be the Banach space consisting of complex measurable functions on $\mathbb{R}^l$ with the norm $\|f\|_p = (\int_{\mathbb{R}^l} |f(x)|^p dx)^{1/p}$. Let $H_{0,p}$ $(1 \leqslant p < \infty)$ be the infinitesimal generator of a C_0-semigroup in the L^p space with a kernel $(4\pi t)^{-l/2} \exp(-|x-y|^2/4t)$. Let V be a measurable function and we use V_p to denote an associated operator in L^p with the domain

$$\mathscr{D}(V_p) = \{ f \in L^p : \textstyle\int_{\mathbb{R}^l} |V(x) f(x)|^p dx < \infty \} .$$

Consider the Schrödinger operator $H_{0,p} + V_p$ acting in L^p space. The requirement of a relative boundness of the operator $V^- \equiv \min\{0, -V\}$ is available in all our results (see Secs. 4–6 below). So we shall give the definition of some perturbation classes in this section.

Definition: Let V be a real valued measurable function. Then $V \in PK$ (pseudo-Kato potential) if and only if there exists $\lambda_0 > 0$ such that

$$\|(H_0 + \lambda)^{-1/2} V (H_0 + \lambda)^{-1/2}\|_{2,2} < 1$$
$$(H_0 \equiv H_{0,2}, \quad V \equiv V_2),$$

for all $\lambda \geqslant \lambda_0$. The number $a = \inf_{\lambda > 0} \|(H_0 + \lambda)^{-1/2} V (H_0 + \lambda)^{-1/2}\|_{2,2}$ is called the $H_0^{1/2}$-bound of the operator V. [$\mathscr{L}(L^p, L^q)$ denotes the space of bounded operators from L^p to L^q, $\mathscr{L}(L^p) \equiv \mathscr{L}(L^p, L^p)$, and $\|\cdot\|_{p,q}$ denotes the norm in $\mathscr{L}(L^p, L^q)$] .

Notice that the inclusion $V \in PK$ implies a possibility of correct construction of the form sum (see, for example, Ref. 6, Chapter VI).

Definition: Let V be a real valued measurable function of $\mathbb{R}^l$. Then $V \in P_p$, $1 \leqslant p < \infty$ (Phillips perturbation) if and only if there exists $\lambda_0 > 0$ such that

$$\|V_p (H_{0,p} + \lambda)^{-1}\|_{p,p} < 1$$

for all $\lambda \geqslant_0$.

Note that $PK_{1 < p < \infty}^{\cup} P_p \subset L^1_{\rm loc}(\mathbb{R}^l)$. Moreover, we shall prove the following.

Proposition 1.1: Let $\lambda > 0$ and $1 \leqslant p < \infty$ be fixed. Suppose V be a real valued function and

$$\|V(-\Delta + \lambda)^{-1}\|_{p,p} \leqslant M . \tag{1.1}$$

Then

$$\|V^s(-\Delta + \lambda)^{-1} |V|^{1-s}\|_{p_s,p_s} \leqslant M , \tag{1.2}$$

where $V^s = |V|^s \operatorname{sign} V$, $1/p_s = 1 - s + (2s-1)/p$, $s \in [0,1]$, $(-\Delta + \lambda)^{-1}$ is a Bessel potential.

Proof: Let $\mathscr{D}$ be a space of simple functions from L^1. The duality of L^p spaces and (1.1) imply

$$\|(-\Delta + \lambda)^{-1} V f\|_{p'} \leqslant M \|f\|_{p'} ,$$
$$\forall f \in \mathscr{D}, \ (1/p) + (1/p') = 1 . \tag{1.3}$$

Define $F(z) = V^z(-\Delta + \lambda)^{-1} |V|^{1-z}$, $z = s + i\sigma$, $\sigma \in \mathbb{R}^1$, $s \in [0,1]$. It is easy to see that map $z \to \langle f, F(z) g \rangle$ (here and further $\langle u,v \rangle = \int_{\mathbb{R}^l} u(x) \overline{v(x)}\, dx$) is holomorphic and uni-

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formly bounded on z in strip $0 \leqslant s \leqslant 1$ for any $f, g \in \mathbb{D}$. Next, (1.1) and (1.3) imply

$$\|F(i\sigma)f\|_{p'} \leqslant \|(-\Delta + \lambda)^{-1}|Vf|\,\|_{p'} \leqslant M\|f\|_{p'},$$

$$\|F(1+i\sigma)f\|_p \leqslant \|V(-\Delta+\lambda)^{-1}f\|_p \leqslant M\|f\|_p, \quad \forall f \in \mathscr{D}, \ \forall \sigma \in \mathbb{R}^1.$$

The latter and the Stein interpolation theorem[7] imply

$$\|F(s)\|_{p_s p_s} \leqslant M, \quad s \in [0,1], \ (1/p_s) = (s/p) + (1-s)/p'. \ \blacksquare$$

Corollary 1.2: $\cup_{1 < p < \infty} P_p \subset PK$.

We shall further give some sufficient conditions in terms of weak L^p spaces which guarantee the validity of $V \in PK$, $V \in P_p$. These conditions are very close to the necessary conditions so that we need to control the value of constants figuring in some fundamental inequalities such as a Strichartz inequality.

2. SOME L^p INEQUALITIES

A function f and $\mathbb{R}^l$ is said in $L^p_w(\mathbb{R}^l) \equiv L^p_w$ written $f \in L^p_w$, if there is a constant $C < \infty$ so that

$$\mu\{x : |f(x)| > t\} \leqslant Ct^{-p} \quad \text{for all } t > 0,$$

where μ is the Lebesque measure. If $f \in L^p_w$, we write

$$\|f\|_{p,w} = \sup_{t>0} (t^p \mu\{x : |f(x)| > t\})^{1/p}.$$

Notice that $\|\cdot\|_{p,w}$ is not a norm since it does not satisfy the triangle inequality.

The following proposition is well known.

Proposition 2.1: $L^p \subset L^p_w$ and $\|f\|_{p,w} \leqslant \|f\|_p$.

Definition: Let f be a nonnegative measurable function on $\mathbb{R}^l$. A function f^* is called the symmetric decreasing rearrangement of f if and only if the following conditions are satisfied:

(1) $f^*(x)$ depends on the $|x|$ only;

(2) $0 < |x_1| < |x_2| \Rightarrow f^*(|x_2|) \leqslant f^*(|x_1|)$;

(3) $\mu\{x : f(x) > t\} = \mu\{x : f^*(x) > t\}$ for all $t > 0$.

We now give a formulation of some known properties of rearrangement which we shall subsequently need (the proofs may be found in Ref. 8, Chap. X or in Ref. 9):

Proposition 2.2: Suppose that $f \geqslant 0$ and $\mu\{x : f(x) > t\} < \infty$ for some $t < \infty$. Then f^* exists and it is unique up to the set of measure zero.

Proposition 2.3: Let $f \geqslant 0$. Then $(f^*)^p = (f^p)^*$.

Proposition 2.4: Let $f, g \geqslant 0$ and $p \in [1,\infty)$, then $\|fg\|_p \leqslant \|f^* g^*\|_p$.

Remark: Obviously, Proposition 2.4 may be generalized to three and more number of functions. In particular

$$\|fg\psi\|_p \leqslant \|f^* g^* \psi^*\|_p. \tag{2.1}$$

Proposition 2.5: Let $f \geqslant 0$. Then $f \in L^p_w$ is equivalent to the following inequality (for a.e. $x \in \mathbb{R}^l$): $f^*(x) \leqslant \Omega_l^{-1/p} \|f\|_{p,w} |x|^{-l/p}$, where $\Omega_l = [2\pi^{l/2}/\Gamma(l+2)/2]$ is the volume of the unit ball in $\mathbb{R}^l$.

The above facts are well known and may be found in Hardy–Littlewood–Polya.[8] The same book contains the classical Riesz theorem about the rearrangement of three functions, which was generalized by S. Sobolev[10] to the multidimensional case.

Theorem (Riesz–Sobolev): Let f, g, h be nonnegative measurable functions on $\mathbb{R}^l$. Then

$$\|f(g * h)\|_1 \leqslant \|f^*(g^* * h^*)\|_1,$$

where $*$ means the convolution.

Subsequently we shall need the following generalization of the Riesz–Sobolev theorem:

Proposition 2.6: Let f, g, h be nonnegative measurable functions on $\mathbb{R}^l$. Then

$$\|f(g * h)\|_p \leqslant \|f^*(g^* * h^*)\|_p \tag{2.2}$$

for any $p \in [1,\infty)$.

Proof: Using inequalities

$$\|f(g * h)\|_1 \leqslant \|f^*(g^* * h^*)\|_1, \qquad \|fg\psi\|_1 \leqslant \|f^* g^* \psi^*\|_1, \tag{2.3}$$

we have

$$\|f(g * h)\psi\|_1 \leqslant \|f^*(g^* * h^*)\,\psi^*\|_1. \tag{2.4}$$

It is clear that (2.4) and the equality

$$\|u\|_p = \sup_{0 \neq \varphi \in L^{p'}} \frac{|\langle u, \varphi\rangle|}{\|\varphi\|_{p'}}, \ \frac{1}{p} + \frac{1}{p'} = 1$$

imply (2.2).

Remark: The inequality (2.2) is a particular case of the general Brascamp–Lieb–Luttinger inequality[11]:

$$\int_{\mathbb{R}^{nl}} \prod_{i=1}^{k} f_i\left(\sum_{j=1}^{n} a_{ij} x_j\right) d^{nl}x \leqslant \int_{\mathbb{R}^{nl}} \prod_{i=1}^{k} f^*\left(\sum_{j=1}^{n} a_{ij} x_j\right) d^{nl}x,$$

where $\mathbb{R}^l \ni x = (x_1, \ldots, x_n)$, $x_j \in \mathbb{R}^l$, $(1 \leqslant j \leqslant n)$; $f_i (1 \leqslant i \leqslant k)$ are nonnegative measurable functions on $\mathbb{R}^l$; a_{ij} are real numbers.

Subsequently we shall need the following notations and formulas:

$$I_\alpha = (-\Delta)^{-\alpha/2}, \quad \alpha < 0$$

is a Riesz potential defined by the formula:

$$(I_\alpha f)(x) = \frac{1}{\gamma(\alpha)} \int_{\mathbb{R}^l} |x - y|^{-l+\alpha} f(y)\,dy,$$

$$\gamma(\alpha) = \frac{2^\alpha \pi^{l/2} \Gamma(\alpha/2)}{\Gamma(l-\alpha)/2}.$$

It is well known that

$$\frac{\gamma(\alpha)\,\gamma(\beta)}{\gamma(\alpha+\beta)} |x|^{-l+\alpha+\beta} = \int_{\mathbb{R}^l} |x-y|^{-l+\alpha} |y|^{-l+\beta}\,dy, \tag{2.5}$$

where $\alpha > 0, \beta > 0, \alpha + \beta < l$.

$\mathscr{F}_\alpha = (1 - \Delta)^{-\alpha/2}$, $\alpha > 0$ is a Bessel potential defined by the formula

$$(\mathscr{F}_\alpha f)(x) = \int_{\mathbb{R}^l} G_\alpha(x-y) f(y)\,dy,$$

where

$$G_\alpha(x)=\frac{1}{(4\pi)^{\alpha/2}\Gamma(\alpha/2)}\int_0^\infty e^{-(\pi|x|^2/\delta)-(\delta/4\pi)}\,\delta^{(-l+\alpha-2)/2}\,d\delta .$$

Lemma 2.7: Let $(T_\alpha f)(x)=|x|^{-\alpha}(I_\alpha f)(x)$, $\alpha>0$ and $1<p<l/2$. Then

$$\|T_\alpha\|_{p,p}\leqslant c(\alpha,p,l), \qquad (2.6)$$

where

$$c(\alpha,p,l)=\frac{\gamma[(l/p)-\alpha]}{\gamma(l/p)}.$$

Proof: Let $\varphi(x)=|x|^{-l/p}$, $\psi(x)=|x|^{-l/p'}$, $(1/p)+(1/p')=1$, $1<p<(l/\alpha)$. It follows from (2.5) that

$$T_\alpha\varphi=c(\alpha,p,l)\,\psi^{p'/p},\; T_\alpha^*\psi=c(\alpha,p,l)\,\varphi^{p/p'},$$

$$(T_\alpha^*=I_\alpha|x|^{-\alpha}).$$

The latter implies (2.6). In fact, let $0\leqslant u\in L^p$, $0\leqslant v\in L^{p'}$ (Since the operator T_α is positivity preserving, we may consider only nonnegative functions). Using Hölder inequality, we obtain

$$0\leqslant\langle T_\alpha u,v\rangle$$

$$=\iint_{R^lR^l}T_\alpha(x,y)\,u(y)\,v(x)\,dx\,dy$$

$$\times\left(\iint_{R^lR^l}T_\alpha(x,y)\,u(y)^p\frac{\psi(x)}{\varphi(y)^{p/p'}}dx\,dy\right)^{1/p}$$

$$\times\left(\iint_{R^lR^l}T_\alpha(x,y)\,v(x)^{p'}\frac{\varphi(y)}{\psi(x)^{p'/p}}dx\,dy\right)^{1/p'}$$

$$=c(\alpha,p,l)\|u\|_p\,\|v\|_{p'}.$$

Hence, $\|T_\alpha\|_{p,p}\leqslant c(\alpha,p,l)$. ■

Remarks: (1) The proof of the inequality $\langle T_\alpha,u,v\rangle\leqslant c(\alpha,p,l)\|u\|_p\|v\|_{p'}$ is based on the tool which is due to I. Schur, G. Hardy, J. Littlewood, and G. Polya, which was formulated in a more abstract form by N. Aronszajn.[12]

(2) Lemma 2.7 was proved in the same say by B. Karlsson[13] in the case $p=2$. Another proof of the lemma was given by I. Herbst.[14]

We shall also need the following.

Lemma 2.8: Let $\chi_n(\cdot)$ be a characteristic function of the set $\{x:n^{-1}\leqslant|x|\leqslant n\}$ and $\alpha>0$, $1<p<l/\alpha$, $\varphi(x)=|x|^{-l/p}$. Put $\varphi_n=\chi_n\,\varphi$. Then

$$\overline{\lim_{n\to\infty}}\|\chi_nT_\alpha(\varphi(1-\chi_n))\|_p<\infty .$$

Proof: We shall further denote values of all nonessential constants by C. Obviously,

$$\mathscr{T}_n\equiv\gamma(\alpha)^p\|\chi_nT_\alpha(\varphi(1-\chi_n))\|_p^p$$

$$=\int_{n^{-1}\leqslant|x|\leqslant n}|x|^{-\alpha p}\left(\int_{\{0<|y|<n^{-1}\}\cup\{n<|y|\}}|y|^{-l/p}|x-y|^{-l+\alpha}dy\right)^p dx$$

$$=\int_{n^{-1}\leqslant|x|\leqslant 2n^{-1}}|x|^{-\alpha p}\left(\int_{\{0<|y|</2n\}\cup\{1/2n\leqslant|y|\leqslant1/n\}\cup\{n\leqslant|y|\}}|x-y|^{-l+\alpha}dy\right)^p dx$$

$$\times\int_{2n^{-1}\leqslant|x|\leqslant n}|x|^{-\alpha p}\left(\int_{\{0<|y|\leqslant1/2n\}\cup\{1/2n\leqslant|y|\leqslant1/n\}\cup\{|y|>n\}}|y|^{-l/p}|x-y|^{-l+\alpha}dy\right)^p dx$$

$$=\mathscr{T}_n^{(1)}+\mathscr{T}_n^{(2)}.$$

Let $2/n<|x|<n$. Then

$$\left\{y:0<|y|<\frac{1}{n}\right\}\subset\left\{y:|x-y|>\frac{|x|}{2}\right\},$$

$$\{y:|y|>2n\}\subset\left\{y:|x-y|>\frac{|y|}{2}\right\},$$

$$\{y:|x-y|<2n\}\subset\{y:|y|<3n\}.$$

Thus

$$\int_{\{0<|y|<n^{-1}\}}|y|^{-l/p}|x-y|^{-l+\alpha}dy$$

$$\leqslant C|x|^{-l+\alpha}\int_{\{0<|y|<n^{-1}\}}|y|^{-l/p}dy$$

$$=C|x|^{-l+\alpha}n^{-l+(l/p)},$$

$$\times\int_{\{2n\leqslant|y|\}}|y|^{-l/p}|x-y|^{-l+\alpha}dy$$

$$\leqslant C\int_{\{2n\leqslant|y|\}}|y|^{-l+\alpha-(l/p)}dy=Cn^{-(l/p)+\alpha},$$

$$\int_{\{n<|x-y|<2n\}}|y|^{-l/p}|x-y|^{-l+\alpha}dy$$

$$\leqslant n^{-l/p}\int_{n<|x-y|<2n}|y|^{-l+\alpha}dy$$

$$=n^{-l/p}\int_{0<|y|<3n}|y|^{-l+\alpha}dy=Cn^{-(l/p)+\alpha}.$$

$$\mathscr{T}_n^{(2)}\leqslant C\int_{2/n\leqslant|x|\leqslant n}|x|^{-\alpha p}(|x|^{-l+\alpha}n^{-l+(l/p)}+n^{-(l/p)+\alpha})^p\,d$$

Using the inequality $(a+b)^p\leqslant2^{p-1}(a^p+b^p)$, $p\geqslant1$, we obtain

$$\mathscr{T}_n^{(2)}\leqslant Cn^{-(l/p)+l}\int_{2/n\leqslant|x|\leqslant n}|x|^{-l/p}dx+Cn^{-l+\alpha p}$$

$$\times\int_{2/n\leqslant|x|\leqslant n}|x|^{-\alpha p}dx.$$

The direct calculations show that

$$\sup_{n\geq 1} \mathcal{T}_n^{(2)} < \infty .$$

By analogy with the above arguments we have

$$\sup_{n\geq 1} \mathcal{T}_n^{(1)} < \infty .$$ ■

Corollary 2.9 [14]: Let $\alpha > 0$, $1 < p < l/\alpha$. Then

$$\|T_\alpha\|_{p,p} = c(\alpha, p, l) .$$

Proof: Notice that

$$\|T_\alpha \varphi_n\|_p > \|\chi_n T_\alpha \varphi_n\|_p > \|\chi_n T_\alpha \varphi\|_p - \|\chi_n T_\alpha (\varphi(1-\chi_n))\|_p$$

(in notations of Lemma 2.8). Hence, using the identity $T_\alpha \varphi = c(\alpha, p, l)\,\varphi$, we obtain

$$\lim_{n\to\infty} \frac{\|T_\alpha \varphi_n\|_p}{\|\varphi_n\|_p} \geqslant c(\alpha, p, l) \overline{\lim_{n\to\infty}} \frac{\|\chi_n T_\alpha (\varphi(1-\chi_n))\|_p}{\|\varphi_n\|_p} .$$

As $\overline{\lim_{n\to\infty}} \|\chi_n T_\alpha (\varphi(1-\chi_n))\|_p < \infty$ by Lemma 2.8 and $\|\varphi_n\|_p \to \infty$, $(n\to\infty)$, so we have

$$\|T_\alpha\|_{p,p} \geqslant \lim_{n\to\infty} \frac{\|T_\alpha \varphi_n\|_p}{\|\varphi_n\|_p} \geqslant c(\alpha, p, l).$$

Thus in view of Lemma 2.7 $\|T_\alpha\|_{p,p} = c(\alpha, p, l)$. ■

If we replace the Riesz potential I_α by the Bessel potential $\mathcal{F}_\alpha$ in the definition of the operator T_α, Corollary 2.9 is also true. Actually, it is easy to see that the norm of the operator $|x|^{-\alpha}(\lambda^2 - \Delta)^{-\alpha/2}$ is invariant under the transformation $x \to \lambda x$.

The main result of the section is

Theorem 2.10: Let $f \in L_w^q$, $g \in L_w^{q'}$, $h \in L^p$, $(1/q) + (1/q') = 1$, $1 < p < q$. Then

$$\|f(g * h)\|_p \leqslant \Omega_l^{-1} \gamma\left(\frac{l}{p} - \frac{l}{q}\right) \|f\|_{q,w} \|g\|_{q',w} \|h\|_p . \tag{2.7}$$

The constant in (2.7) is best possible.

Proof: Using Theorem 2.6, Proposition 2.5, and Corollary 2.9 we obtain:

$$\begin{aligned}\|f(g*h)\|_p &\leqslant \| |f|^*(|g|^* * |h|^*)\|_p \\ &\leqslant \Omega_l^{-1} \gamma\left(\frac{l}{q}\right) \|f\|_{q,w} \|g\|_{q,w} \|T_{l/q} |h|^*\|_p \\ &\leqslant \Omega_l^{-1} \gamma\left(\frac{l}{q}\right) c\left(\frac{l}{q} p, l\right) \|f\|_{q,w} \|g\|_{q',w} \|h\|_p \\ &= \Omega_l^{-1} \gamma\left(\frac{l}{p} - \frac{l}{q}\right) \|f\|_{q,w} \|g\|_{q',w} \|h\|_p .\end{aligned}$$

We now show that the constant in (2.7) is optimal. In fact, putting $f = |x|^{-l/q}$, $g = |x|^{-l/q'}$, we obtain

$$\|f(g*h)\|_p = \gamma\left(\frac{l}{q}\right) \|T_{l/q} h\|_p \leqslant \gamma\left(\frac{l}{q}\right) c\left(\frac{l}{q}, p, l\right) \|h\|_p$$

and Corollary 2.9 implies that the last inequality is optimal. ■

Corollary 2.11: Let $f \in L_w^{l/\alpha}$, $p \in [1, (l/\alpha)]$. Then

$$\|f I_\alpha u\|_p \leqslant \Omega_l^{-\alpha/l} c(\alpha, p, l) \|f\|_{l/\alpha, w} \|u\|_p .$$

Corollary 2.12: (*Strichartz inequality*): Let $1 < p < l/\alpha$. Then

$$\|fu\|_p \leqslant \Omega_l^{-\alpha/l} c(\alpha, p, l) \|f\|_{l/\alpha, w} \|u\|_{\mathcal{L}_\alpha^p} \tag{2.8}$$

for any $u \in \mathcal{L}_\alpha^p$. ($\mathcal{L}_\alpha^p$ is the space of Bessel potentials.[10])

Remarks: (1) The inequalitites (2.7) and (2.8) have been proved by R. Strichartz,[5] who used the Hunt's and Marcinkiewicz's interpolation theorems. The mean of Theorem 2.10 and Corollary 2.12 consists in calculating the *best* constants in these inequalities

(2) In the case $\alpha = 1$ the Strichartz inequality may be written in the other form, i.e., we can replace $\|u\|_{\mathcal{L}_\alpha^p}$ by $\|Du\|_p = \|(\Sigma_{i=1}^l |\partial u/\partial x_i|^2)^{1/2}\|_p$. In this situation W. Faris[9] calculated the best constant in the Strichartz inequality and extended it on the case $p = 1$:

$$\|fu\|_p \leqslant \Omega_l^{-1/l} \frac{p}{l-p} \|f\|_{l,w} \|Du\|_p , \quad 1 \leqslant p < l , \tag{2.8a}$$

for any sufficiently smooth u, which decreases at the infinity sufficiently rapidly.

Notice that consideration of $p = 1$ is impossible in our problem.

Using (2.8) it is not difficult to prove some classical inequalities, but the constants, which will be obtained, are not optimal.

Corollary 2.13 (*homogeneous Sobolev inequality*): Let $1 < p < l/\alpha$. Then

$$\|u\|_q \leqslant \Omega_l^{-\alpha/l} c(\alpha, p, l) \|(-\Delta)^{\alpha/2} u\|_p, \quad (1/q) = (1/p) - (\alpha/l) , \tag{2.9}$$

for all sufficiently smooth u, which decrease at infinity sufficiently rapidly.

Proof: Putting $f = u^*$, $k = \alpha p/(l - \alpha p)$ in (2.8) and using the inequality

$$\|u\|_{p,w} \leqslant \|u\|_p , \tag{2.10}$$

we have

$$\|fu\|_p = \|u\|_{(k+1)p}^{k+1} \leqslant \Omega_l^{-\alpha/l} c(\alpha, p, l) \|u\|_{pl/(l-\alpha p)}^k \|(-\Delta)^{\alpha/2} u\|_p .$$

The latter is equivalent to (2.9).

Remarks: (1) Since we used (2.10) in the proof of Corollary 2.13, the constant in (2.9) is not optimal.

(2) If $\alpha = 1$, the inequality (2.9) as well as the Strichartz inequality may be rewritten in the form [see Remark (2) below Corollary 2.13]:

$$\|u\|_q \leqslant \text{const} \|Du\|_p , (1/q) = 1/p - (\alpha/l) , \quad 1 < p < l . \tag{2.10a}$$

Using (2.8a) and an argument analogous to the proof of Corollary 2.13, W. Faris[9] proved that one may put const $= \Omega_l^{-1/l} p/(l-p)$ in the inequality (2.10a), but this constant is not optimal. The value of the optimal constant was computed by T. Aubin[15] and G. Talenti[16]:

$$\text{const} = \pi^{-1/2} l^{-1/p} \left(\frac{p-1}{l-p}\right)^{1-(1/p)} \times \left\{\frac{\Gamma[1 + (l/2)]\Gamma(l)}{\Gamma(l/p)\Gamma[1 + l - (l/p)]}\right\}^{1/l} .$$

Moreover, the following question was investigated by A. Alvino[17]: What is the value of the best constant in Sobolev's inequality if we replace L^p spaces by Lorentz spaces $L(p,q)$. He proved the following inequality:

$$\|u\|_{q,v} \leqslant \Omega_l^{-1/l} \frac{p}{l-p} \|Du\|_{p,v},$$

$$\frac{1}{q} = \frac{1}{p} - \frac{1}{l}, \quad 1 \leqslant p < l, \ 1 \leqslant v \leqslant p \qquad (2.10b)$$

The other form of the inequality (2.9) is

Corollary 2.14 (*L^p-inequality for Riesz potentials*): Let $1 < p < l/\alpha$, $0 < \alpha < l$, $(1/q) = (1/p) - (\alpha/l)$. Then

$$\|I_\alpha f\|_q \leqslant \Omega_l^{-\alpha/l} c(\alpha, p, l) \|f\|_p. \qquad (2.11)$$

Remark: The (2.11) is valid if we replace I_α by $\mathscr{F}_\alpha$ [see Remark (3) to Lemma 2.7]. By analogy, (2.9) is valid if we replace $(-\Delta)^{\alpha/2}$ by $(\lambda - \Delta)^{\alpha/2}$, $\mathrm{Re}\lambda > 0$.

Corollary 2.15 (*generalized Young's inequality*): Let $f \in L^p_w$, $g \in L^q$. Then

$$\|f * g\|_r \leqslant \Omega_l^{-1} \gamma(l/p') c(l/p', q, l) \|f\|_{p,w} \|g\|_q,$$

where $(1/p) + (1/p') = 1$, $(1/q) + (1/q') = 1$, $1 < p,q,r < \infty$, $1 + (1/r) = (1/p) + (1/q)$.

Proof: Obviously, we can consider $f, g \geqslant 0$ only. Since $\|f * g\|_r \leqslant \|f^* * g^*\|_r$ (see Lemma 2.6), using Proposition 2.5 and (2.11), we obtain

$$\begin{aligned}\|f * g\|_r &\leqslant \Omega_l^{-1/p} \|f\|_{p,w} \| \, |x|^{-l/p} * g^*\|_r \\ &= \Omega_l^{-1/p} \gamma\left(\frac{l}{p'}\right) \|f\|_{p,w} \| \Omega_{l/p'} g^*\|_r \\ &\leqslant \Omega_l^{-1/p} \gamma\left(\frac{l}{p'}\right) \Omega_l^{-1/p'} c \\ &\quad \times \left(\frac{l}{p'}, q, l\right) \|f\|_{p,w} \|g\|_q. \qquad \blacksquare\end{aligned}$$

Remark: Corollary 2.15 clearly implies the classical Young's inequality, but the constant in this case is not optimal. The question about the best constant in the Young's inequality and a related question about best constants in the Hausdorff Young's inequality is due to K.I. Babenko[18] and was completely investigated by W. Becner,[19] and H.J. Brascamp and E.H. Lieb.[20]

Corollary 2.16 (*Sobolev inequality*): Let $f \in L^p$, $h \in L^r$. Then

$$\iint_{\mathbb{R}^l \mathbb{R}^l} \frac{|f(x)| \, |h(y)|}{|x-y|^\lambda} dx\, dy \leqslant \gamma(l-\lambda) \Omega_l^{-(l-\lambda)/l} c(l-\lambda, r, l) \|f\|_p \|h\|_r, \qquad (2.12)$$

where

$$(1/p) + (1/r) + (\lambda/l) = 2, \quad 0 < \lambda < l, \quad 1 < p,r < \infty.$$

Proof: Using the Hölder inequality and (2.11) we have

$$\begin{aligned}&\iint_{\mathbb{R}^l \mathbb{R}^l} \frac{|f(x)| \, |h(y)|}{|x-y|^\lambda} dx\, dy \\ &\equiv \gamma(l-\lambda) \|f I_{l-\lambda} |h| \|_1 \leqslant \gamma(l-\lambda) \|f\|_p \|I_{l-\lambda} |h| \|_{p'} \\ &\leqslant \gamma(l-\lambda) \Omega_l^{-(l-\lambda)/l} c(l-\lambda, r, l) \|f\|_p \|h\|_r,\end{aligned}$$

where

$$(1/p) + (1/p') = 1, \quad (1/p') = (1/r) - (l-\lambda)/l. \qquad \blacksquare$$

As we noted, the constants in Corollaries 2.14–2.16 are not the best possible. But we can prove some inequalities which are the generalization of these corollaries (in some sense) and have optimal constants.

Theorem 2.17: Let $0 < \alpha < l$, $1 < p < l/\alpha$, $(1/q) = (1/p) - (\alpha/l)$. Then

$$\|I_\alpha f\|_q \leqslant \Omega_l^{-\alpha/l} c(\alpha, p, l) \|f\|_{p,w}^{\alpha p/l} \|f\|_p^{1-(\alpha p/l)}, \quad \forall f \in L^p. \qquad (2.13)$$

The constant $\Omega_l^{-\alpha/l} c(\alpha, p, l)$ is best possible.

Proof: Let $0 \leqslant f \in L^p$. Put $t = \alpha p/l$, then we have

$$\begin{aligned}\|I_\alpha f\|_q &\leqslant \|I_\alpha f^*\|_q \\ &\leqslant \Omega_l^{-t/p} \|f\|_{p,w}^t \|I_\alpha |x|^{-\alpha} (f^*)^{1-t}\|_q \\ &= \Omega_l^{-t/p} \|f\|_{p,w}^t \|T_\alpha^* (f^*)^{1-t}\|_q \\ &\leqslant \Omega_l^{-t/p} \|f\|_{p,w}^t \|T_\alpha^*\|_{q,q} \|f\|_{q(1-t)}^{1-t} \\ &= \Omega_l^{-t/p} \|f\|_{p,w}^t c(\alpha, q', l) \|f\|_p^{1-t}, \quad (1/q) + (1/q') = 1\end{aligned}$$

Notice that $q(1-t) = p$ and $c(\alpha, q', l) = c(\alpha, p, l)$. Thus (2.13) is proved.

Let us show that the constant $\Omega_l^{-\alpha/l} c(\alpha, p, l)$ is the best possible. Let $f_n(x) = |x|^{-l/p} \chi_n(x)$, where χ_n is a characteristic function of the set $\{x: n^{-1} \leqslant |x| \leqslant n\}$. It is clear that

$$(I_\alpha f_n)(x) = (T_\alpha^* f_n^{1-t})(x) \quad \text{and} \quad \lim_{n \to \infty} \|f_n\|_{p,w} = \Omega_l^{1/p}.$$

Hence, using Corollary 2.9, we have

$$\lim_{n\to\infty} \frac{\|I_\alpha f_n\|_q}{\|f_n\|_p^{1-t}} = \Omega_l^{-\alpha/p} \lim_{n\to\infty} \left(\|f_n\|_{p,w}^t \frac{\|T_\alpha^* f_n^{1-t}\|_q}{\|f_n\|_p^{1-t}} \right) = c(\alpha, p, l).$$

The latter implies that the constant $\Omega_l^{-\alpha/l} c(\alpha, p, l)$ is the best possible.

Theorem 2.18: Let $f \in L^p$, $h \in L^q$, $1 + (1/r) = (1/p) + (1/q)$, $1 < p,q,r < \infty$, $0 \leqslant \epsilon \leqslant 1$. Then

$$\begin{aligned}\|f * h\|_r &\leqslant \Omega_l^{-1} \gamma(l/p') c((l/p'), r', l) \|f\|_{p,w}^{1-(p/r)\epsilon} \\ &\quad \times \|f\|_p^{(p/r)\epsilon} \|h\|_{q,w}^{1-(q/r)(1-\epsilon)} \|h\|_q^{(q/r)(1-\epsilon)} \qquad (2.14)\end{aligned}$$

The constant $\Omega_l^{-1} \gamma(l/p' c)((l/p'), r', l)$ is the best possible.

Proof: As usually we consider $f, h \geqslant 0$. Using (2.13), we have

$$\begin{aligned}\|f * h\|_r &\leqslant \|f^* * h^*\|_r \\ &\leqslant \Omega_l^{-1/p} \|f\|_{p,w} \| \, |x|^{-l/p} * h^*\|_r \\ &= \Omega_l^{-1/p} \gamma(l/p') \|f\|_{p,w} \| I_{l/p'} h^*\|_r \\ &\leqslant \Omega_l^{-1/p} \gamma(l/p') c((l/p'), r', l) \|f\|_{p,w} \|h\|_{q,w}^{q/p'} \|h\|_q^{1-(q/p')}.\end{aligned}$$

By analogy,

$$\|f * h\|_r \leqslant \Omega_l^{-1} \gamma(l/q') c((l/q'), r', l) \|h\|_{q,w} \|f\|_{p,w}^{p/q'} \|f\|_p^{1-(p/q')}.$$

(2.14) now follows from the last inequalities and identities

$$\|f * h\|_r = \|f * h\|_r^\epsilon \|f * h\|_r^{1-\epsilon},$$

$$\gamma(l/p') c((l/p'), r', l) = \gamma(l/q') c((l/q'), r', l).$$

Putting $f_n(x) = |x|^{-l/p} \chi_n(x)$, $h_n(x) = |x|^{-l/q} \chi_n(x)$, it is easy to show that

$$\lim_{n\to\infty} \frac{\|f_n * h_n\|_r}{\|f_n\|_{p,w}^{1-(p/r)\epsilon}\|f_n\|_p^{(p/r)\epsilon}\|h_n\|_{q,w}^{1-(q/r)(1-\epsilon)}\|h_n\|_q^{(q/r)(1-\epsilon)}} = \Omega_l^{-1}\gamma(l/p')\, c(l/p',r',l).$$

The latter implies that the constant in (2.14) is optimal.

Theorem 2.19: Let $f\in L^p$, $h\in L^q$, $0<\lambda<l$, $1<p,q<\infty$, $(1/p)+(1/q)+(\lambda/l)=2, 0 \leqslant \epsilon \leqslant 1$. Then

$$\iint_{\mathbb{R}^l\mathbb{R}^l} \frac{|f(x)|\,|h(y)|}{|x-y|^\lambda}\,dx\,dy \leqslant \Omega_l^{-1+(\lambda/l)}\gamma(l-\lambda)\,c(l-\lambda,p,l) \times \|f\|_{p,w}^{(l-\lambda)p\epsilon}\|f\|_p^{1-[(l-\lambda)p\epsilon/l]}\|h\|_{q,w}^{(l-\lambda)q(1-\epsilon)/l} \times \|h\|_q^{1-[(l-\lambda)q(1-\epsilon)/l]}. \tag{2.15}$$

The constant $\Omega_l^{-1+(\lambda/l)}\gamma(l-\lambda)\,c(l-\lambda,p,l)$ is the best possible.

Proof: Let $0\leqslant f\in L^p$, $0\leqslant h\in L^q$. Using Theorem 2.6 and the Hölder inequality, we have

$$\langle f, I_{l-\lambda} h\rangle \leqslant \|f\|_p\,\|I_{l-\lambda} h\|_{p'},\quad (1/p)+(1/p')=1, \tag{2.16}$$

$$\langle I_{l-\lambda} f, h\rangle \leqslant \|h\|_q\,\|I_{l-\lambda} f\|_{q'},\quad (1/q)+(1/q')=1. \tag{2.17}$$

The inequality (2.15) follows now from (2.16), (2.17), the identity

$$\langle f, I_{l-\lambda} h\rangle = \langle f, I_{l-\lambda} h\rangle^\epsilon \langle I_{l-\lambda} f, h\rangle^{1-\epsilon},$$

and Theorem 2.17. The proof that the constant is optimal is analogous to the above proofs. ■

Proof: In the one-dimensional case with $\epsilon = 1/\lambda q'$ the inequality (2.15) was proved by V.I. Levin.[21] Levin's proof is based essentially on the conditions $l=1$, $\epsilon = 1/\lambda q'$, and his proof has been reduced to the known inequalities for double numerical series. The above proved inequality (2.15) is basically a generalization of Levin's result, and in the case $l=1$, $\epsilon = 1/\lambda q'$, it appears to be its new proof.

3. SOME SUFFICIENT CONDITIONS FOR $V\in P_p$, $V\in PK$

If we assume $V\in L_w^{l/2}(\mathbb{R}^l)$, then using Corollary 2.11 we can give the following sufficient conditions for the validity of the inclusions $V\in PK$ or $V\in P_p$.

Proposition 3.1: Let $l\geqslant 3$, $1<p<l/2$, and $0<\beta<((l-2)/2)^2$. Suppose that $V\in L_w^{l/2}$. Then

$$(1)\ \|V\|_{l/2,w} < \Omega_l^{2/l}\left(\frac{l-2}{2}\right)^2 \Rightarrow V\in PK;$$

$$(2)\ \|V\|_{l/2,w} < \Omega_l^{2/l}\beta \Rightarrow V\in \bigcap_{p_-(\beta)<p<p_+(\beta)} P_p,$$

where

$$p_\pm(\beta) = \frac{l(l+2\pm\sqrt{(l-2)^2-4\beta})}{2(\beta+2l)}.$$

A comparison of the assertions (1) and (2) of Proposition 3.1 allows us to formulate the following.

Conclusion: The sufficient conditions for the inclusions $V\in PK$ and $V\in P_{2l/(l+2)}$ given in terms of the $\|\cdot\|_{l/2,w}$-norm coincide.

Moreover, the above sufficient conditions are very close to the necessary conditions. Evidently, it is valid the following.

Conjecture: If $l\geqslant 3$, then $PK\subset L_{w,\mathrm{loc}}^{l/2}(\mathbb{R}^l)$.

Remark: The proof of the conjecture seems to be difficult. But there is a more narrow problem which is also open. If $l=3$, there is defined the Rollnik class R, which contains potentials obeying the following inequality

$$\iint_{\mathbb{R}^l\mathbb{R}^l} \frac{|V(x)|\,|V(y)|}{|x-y|^2}\,dx\,dy < \infty.$$

It is known that $R\subset PK$ (see Ref. 22) but the $R\subset L_{w,\mathrm{loc}}^{3/2}$ is not proved. Proposition 3.1 gives sufficient conditions for $V\in P_p$, $1<p<l/2$. But there exists an interesting class P_1, which was completely investigated in Ref. 23. The last problem is more simple, because we write the inequality

$$\sup_{x\in\mathbb{R}^l}\int_{\mathbb{R}^l} \frac{|V(y)|\,e^{-\varkappa|x-y|}}{|x-y|^{l-2}}\,dy < \infty \quad (\text{for some } \varkappa\geqslant 0), \tag{3.1}$$

which gives necessary and sufficient conditions for $V\in P_1$.

In particular, (3.1) implies

$L^p + L^\infty \subset P_1$ for any $p>l/2$. Notice that if $1<p<l/2$

$$L^{l/2} + L^\infty \subset P_p \tag{3.2}$$

(see, for example Ref. 23), but in the case $p=1$ the (3.2) is false. This can be easily shown if we consider the potential

$$V(x) = \frac{\chi(x)}{|x|^2 \ln|x|^{-1}},$$

where $\chi(x)$ is a characteristic function of the ball $\{x: |x|\leqslant 1/2\}$.

4. PERTURBATION OF SEMIGROUP GENERATORS

Before investigating spectral properties of the operator $-\Delta + V$ we shall prove some properties of the semigroup generated by this operator.

Remind that $H_{0,p}$ is a generator of the C_0-semigroup in L^p with an integral kernel $(4\pi t)^{-l/2}\exp(-|x-y|^2/4t)$. and V_p is a multiplicative operator associated with the real values measurable function $V(x)$ with a domain $\mathscr{D}(V_p) = \{f\in L^p: Vf\in L^p\}$.

Lemma 4.1: Suppose that $V_p\in P_p$. Then the operator sum $H_{0,p}+V_p$ is a generator of the quasi-bounded holomorphic semigroup in L^p.

Proof: The unperturbed operator $H_{0,p}$ is a generator of the bounded semigroup in L^p, which is holomorphic in the sector $\{z: |\arg z|<\pi/2\}$, so that for any $\epsilon>0$ there is $M_\epsilon<\infty$ such that $\|(H_{0,p}+z)^{-1}\|_{p,p}\leqslant M_\epsilon/|z|$ for any $z\in\Gamma_\epsilon \equiv \{z: |\arg z|<\pi-\epsilon\}$.

Next, the definition of P_p implies

$$\|V_p(H_{0,p}+\lambda)^{-1}\|_{p,p}<1 \quad \text{for all } \lambda\geqslant\lambda_0>0.$$

Let $z\in\Gamma_\epsilon$. Obviously, there exist $\theta_\epsilon\in(0,1)$ obeying the condition $\mathrm{Re}\sqrt{z+\lambda}\geqslant\sqrt{\lambda\theta_\epsilon}$ for all $z\in\Gamma_\epsilon$, $\lambda\geqslant\lambda_0$. It follows from the explicit form of $(H_{0,p}+z)^{-1}$ that

$$|V_p(H_{0,p}+z+\lambda)^{-1}f| \leqslant |V_p|(H_{0,p}+\lambda\theta_\epsilon)^{-1}|f|, \forall f\in L^p,$$

so that $\|V_p(H_{0p}+z+\lambda)^{-1}\|_{p,p}\leqslant\|V_p(H_{0,p}+\lambda\theta_\epsilon)^{-1}\|_{p,p}<1$ for any $\lambda\geqslant\lambda_0/\theta_\epsilon$. Now it is clear that the Neumann series for the operator $(H_{0,p}+V_p+z+(\lambda_0/\theta_\epsilon))$,$^{-1}$ $z\in|\epsilon$ converges and

$$\|(H_{0,p}+V_p+z+(\lambda_0/\theta_\epsilon))^{-1}\|_{p,p}\leqslant M'/|z+(\lambda_0/\theta_\epsilon)|,$$

where

$$M'=\frac{M_\epsilon}{1-\|V_p(H_{0,p}+\lambda_0)^{-1}\|_{p,p}}.$$

Thus $H_{0,p}+V_p$ with the domain $\mathscr{D}(H_{0,p}+V_p)=\mathscr{D}(H_{0,p})$ is a generator of the quasi-bounded semigroup and $\exp(-t(H_{0,p}+V_p))$ is holomorphic on $\{z:|\arg z|<\pi/2\}$.

Notice that if $\lambda_0=0$, then $\exp(-t(H_{0,p}+V_p))$ is a bounded holomorphic semigroup, since

$$\|(H_{0,p}+V_p+z)^{-1}\|_{p,p}\leqslant M'/|z|,\quad z\in\Gamma_\epsilon. \qquad ■$$

Consider now the self-adjoint (bounded from below) operator A in L^2. Using the operator we can construct a family of operators acting in L^p spaces. It may be done as follows. Consider the semigroup $\epsilon(t)=(e^{-tA}\upharpoonright L^2\cap L^p)^\sim$ in the L^p space, where $\sim$ is a closure of the operator. (We assume that the construction of such a semigroup is possible!) and let A_p be a generator of $\epsilon(t)$. If A is the form sum $H_0\dotplus V$, then the following theorem is valid.

Theorem 4.2: Let $V=V^+-V^-$, $V^\pm\geqslant 0$. Suppose

(1) $V^+\in L^q_{\rm loc}(\mathbb{R}^l\setminus S)$, where $q\in[1,\infty)$ and S is a closed set of the Lebesque measure zero;

(2) $V^-\in P_q$.

Then the definition of the operator $(H_0\dotplus V)_q$ is possible and

$$(H_0\dotplus V)_q\supset(H_{0,q}+V_q)\upharpoonright C_0^\infty(\mathbb{R}^l\setminus S). \tag{4.1}$$

Proof: It follows from the condition (2) that $(H_{0,q}-V_q^-)$ is a generator of the holomorpic semigroup in L^q (see Lemma 4.1). Moreover, $P_q\subset PK$ so that the definition of the form sum $H_0\dotplus(V^+-V^-)$ is possible. Let $V^+_{(n)}$ is a truncated operator corresponding to V, so

$$V^+_{(n)}(x)=\begin{cases}V^+(x) & \text{if } V^+(x)\leqslant n,\\ 0 & \text{if } V^+(x)>n,\end{cases}\qquad n=1,2,\cdots.$$

Introduce the notations

$$C_{(n)}=H_0\dotplus(V^+_{(n)}-V^-),\quad \mathscr{D}(C_{(n)})=\mathscr{D}(H_0\dotplus(-V^-)),\quad C=H_0\dotplus V,$$

$$C_{q,(n)}=H_{0,q}-V_q^-+V^+_{(n)},\quad \mathscr{D}(C_{q,(n)})=\mathscr{D}(H_{0,q}).$$

Notice that

$$C_{(n)}\underset{L^2}{\overset{R}{\to}}C \text{ (strong resolvent convergent in } L^p) \tag{4.2}$$

(see Ref. 23).

On the other hand, we have (see Ref. 23)

$$s-L^q-\lim_n(\lambda+C_{q,(n)})^{-1}\text{ exists for }\forall\lambda\geqslant\lambda_0>0, \tag{4.3}$$

$$s-L^q=\lim_{\alpha\downarrow 0}(1+\alpha C_{q,(n)})^{-1}=1 \text{ uniformly on } n=1,2,\cdots, \tag{4.4}$$

(4.3), (4.4) and the Trotter–Kato theorem (see, for example, Ref. 6, Chapter IX) imply

$$C_{q,(n)}\underset{L^q}{\overset{R}{\to}}C_q, \tag{4.5}$$

where C_q is a generator of some quasi-bounded C_0-semigroup in L^q. Combining (4.2) and (4.5) we obtain

$$e^{-tC_q}|L^2\cap L^q=e^{-tC}|L^2\cap L^q.$$

Thus

$$e^{-tC_q}=(e^{-tC}|L^2\cap L^q)^\sim\equiv e^{-t(H_0\dotplus V)_q}.$$

Let us now show that

$$C_qR_m(C_q)\varphi=R_m(C_q)(H_{0,q}+V_q^+-V_q^-)\varphi,$$
$$\varphi\in C_0^\infty(\mathbb{R}^l\setminus S), \tag{4.6}$$

where $R_m(C_q)=(\lambda+m^{-1}C_q)^{-1}$, $m=1,2,\cdots$.

It is clear that (4.5) is equivalent to

$$C_{q,(n)}R_m(C_{q,(n)})\underset{L^q}{\overset{s}{\to}}C_qR_m(C_q)\quad(n\to\infty), \tag{4.7}$$

where $\underset{L^q}{\overset{s}{\to}}$ means a strong L^q convergent.

On the other hand, using the estimate $\sup_{m\geqslant 1}\|R_m(C_{q,(n)})\|_{q,q}<\infty$, we have

$$C_{q,(n)}R_m(C_{q,(n)})\varphi$$
$$=R_m(C_{q,(n)})C_{q,(n)}\varphi\underset{L^q}{\overset{s}{\to}}R_m(C_q)(H_{0,q}+V_q^+-V_q^-)\varphi$$

for any $\varphi\in C_0^\infty(\mathbb{R}^l\setminus S)$.

Thus (4.6) is proved. Then, putting $m\to\infty$, we obtain

$$\|(R_m(C_q)-1)(H_{qq}+V^+-V^-)\varphi\|_q\to 0,\quad \forall\varphi\in C_0^\infty(\mathbb{R}^l\setminus S).$$

The latter, (4.7) and the fact that C_q is closed imply $C_0^\infty(\mathbb{R}^l\setminus S)\subset\mathscr{D}(C_q)$ and

$$C_q\supset(H_{0,q}+V^+-V^-)|C_0^\infty(\mathbb{R}^l\setminus S).$$

Theorem 4.2 is proved. ■

Remarks: (1) Theorem 4.2 may be extended to a more general situation, that is, the operator H_0 may be replaced by the general self-adjoint operator A such that e^{-tA} is the holomorphic positivity preserving the semigroup in L^1,

$$\bigcap_{1<q<\infty}\mathscr{D}(A_q)\supset C_0^\infty(\mathbb{R}^l\setminus S);$$

A_q-C_q is a generator of the holomorphic semigroup in L^q. Moreover, if $q>1$ the analyticity of e^{-tA} in L^1 is a superfluous condition, because the analyticity of e^{-tA} in L^q is a consequence of the Stein interpolation theorem.

(2) Theorem 4.2 was proved earlier by Yu.A. Semenov[24] for the case $V^-=0$.

5. THE FIRST SPECTRAL PROBLEM FOR OPERATOR $-\Delta+V$

Using the results of the above sections we shall give here some conditions which yield the positive solution of the first spectral problem for the operator $-\Delta\dotplus V$ in the L^p scale.

Theorem 5.1: Let $\beta(p)=[l(p-1)(l-2p)]/p^2$, $1<p<l/2$. Suppose $V=V^+-V^-$, $V^\pm\geqslant 0$ and

(1) $V\in L^p_{\rm loc}(\mathbb{R}^l)$;

(2) $\|V^-\|_{l/2,w}<\Omega_l^{2/l}\beta(p)$.

Then the operator $\widehat{H}_p=(-\Delta+V)\upharpoonright C_0^\infty(\mathbb{R}^l)$ is closable and its closure is a generator of the quasi-bounded holomorphic semigroup. In particular, if $l\geqslant 5$, $p=2$, $\widehat{H}_2$ is essentially self-adjoint. Moreover, if $l\geqslant 5$, $V\in L^2_{\rm loc}(\mathbb{R}^l)$, $\|\overline{V}\|_{l/2,w}\leqslant \Omega_l^{2/l}\beta(2)$, $\widehat{H}_2$ is essentially self-adjoint.

Proof: The condition (2) and Proposition 3.1 imply $V^-\in P_p$ and, consequently, $V^-\in PK$, so that the form sum $H=H_0+(V^+-V^-)$ is correctly defined. Furthermore, the operator $(-\Delta+V^+)\upharpoonright C_0^\infty(\mathbb{R}^l)$ is closable by the Lumer–Phillips theorem[25] (we denote its closure by H_p^+). Since the Davies–Faris lemma Ref. 26, Theorem X.31 gives

$$\|V_p^-(H_p^++\lambda)^{-1}\|_{p,p}\leqslant\|V_p^-(H_{0,p}+\lambda)^{-1}\|_{p,p}<1,$$

$\widehat{H}_p$ is also closable (see Ref. 6, Sec. IV.1). Using arguments based on Kato's inequality it is not difficult to show (see Ref. 24) that $(\widehat{H}_p+1)C_0^\infty(\mathbb{R}^l)$ is dense in L^p, so that the closure of $\widehat{H}_p$ coincides with H_p. Now we shall show the analyticity of $\exp(-tH_p)$.

Obviously, $\exp(-tH)$ is a quasi-bounded holomorphic semigroup in L^2. Suppose now $p>2$. Since the condition (2) turns out to be a strict inequality, from Proposition 3.1 follows that there exists $\epsilon>0$ such that $V^-\in P_{p+\epsilon}$. Hence (see the proof of Theorem 4.2), the operator (H_0+V) is a generator of the quasi-bounded holomorphic semigroup in $L^{p+\epsilon}$. [The assertion of Theorem 4.2 about the validity of (4.1) may be false, because it is possible that $\mathscr{D}(V_{p+\epsilon})\cap C_0^\infty(\mathbb{R}^l)=\{0\}$, but the quasi-boundnes of $\exp(-t(H_0+V)_q)$ is clearly true.]

Thus the H_0+V generates a quasi-contraction holomorphic semigroup in L^2 and a quasi-bounded semigroup in $L^{p+\epsilon}$, so the Stein interpolation theorem implies the analyticity of $\exp(-t(H_0+V)_q)$ in L^p. The consideration of the case $p<2$ is analogous, but we need to replace $p+\epsilon$ on $p-\epsilon$.

Consider now the condition $\|V^-\|_{l/2,w}\leqslant\Omega_l^{2/l}\beta(2)$. It implies

$$\|V^-u\|_2\leqslant\|H_0u\|_2,\quad\forall u\in\mathscr{D}(H_0).$$

So Wüst's theorem gives a significant self-adjointness of H_0-V^- on any core of the operator H_0, in particular, on $C_0^\infty(\mathbb{R}^l)$. Essential self-adjointness of the operator $\widehat{H}_0$ follows from the Davies–Faris lemma and known results on the self-adjointness of $-\Delta+V^+$. ■

Remark: Theorem 5.1 and all further results may be generalized by a trivial way in the case $V^-=V_1^-+V_2^-$, where V_1^- obeys the condition (2) of Theorem 5.1, and $V_2^-\in L^\infty$.

Now consider the case when V^- has a non-L^p-integrable singularity in one point only. It allows one to weaken the condition (2) of Theorem 5.1.

Theorem 5.2: Let $l\geqslant 2$, $p\in[1,\infty)$. Suppose that

(1) $V\in L^p_{\rm loc}(\mathbb{R}^l\setminus\{0\})$;

(2) $V\geqslant\beta(p)|x|^{-2}$. Put $\widehat{H}_p=(-\Delta+V)\upharpoonright C_0^\infty(\mathbb{R}^l\setminus\{0\}):L^p\to L^p$. Then (a) $\text{Ran}(\widehat{H}_p+1)$ is dense in L^p; (b) If $p>2l/(l+2)$, $l\geqslant 3$, the operator $\widehat{H}_p$ is closable and the closure generates the quasi-bounded holomorphic semigroup e^{-tH_p}; (c) If $p\geqslant(l/2)$, $l\geqslant 2$ the operator H_p generates contraction C_0-semigroup e^{-tH_p}.

Proof: (a) Suppose that (a) is not true. Then there exists $h\in L^{p'}$, $(1/p)+(1/p')=1$, $\|h\|_{p'}=1$, such that $\langle(\widehat{H}_p+1)u,h\rangle=0$ for any $u\in C_0^\infty(\mathbb{R}^l\setminus\{0\})$.

So $(-\Delta+V+1)h=0$ (in a distributional sense), or $\Delta h=(V+1)h$. Hence, $h\in L^1_{\rm loc}(\mathbb{R}^l\setminus\{0\})$, $\Delta h\in L^1_{\rm loc}(\mathbb{R}^l\setminus\{0\})$ and so we can apply Kato's inequality (see Ref. 26, p. 183):

$$\Delta|u|\geqslant\text{Re}[(\text{sign}u)\Delta u]$$
$$\times[\text{in distributional sense on } C_0^\infty(\mathbb{R}^l\setminus\{0\})].$$

Thus

$$\Delta|h|\geqslant\text{Re}[(\text{sign}h)\Delta h]=\text{Re}[(\text{sign}h)(V+1)h]$$
$$=(V+1)|h|\geqslant(-\beta(p)|x|^{-2}+1)|h|.$$

So,

$$\int_{\mathbb{R}^l}|h|(-\Delta-\beta(p)|x|^2+1)\varphi\,dx\leqslant 0,\quad\forall\varphi\in C_0^\infty(\mathbb{R}^l\setminus\{0\}).$$

Introduce the functions

$$\phi(s)=|x|^ke^{-|x|},\ k=1-(l/2)+|(l/2)-(l/p)+1|,$$
$$X(x)=|x|^{-1}\phi(x)(1+|l-2-(2l/p)|).$$

Clearly, $0<X\in L^p$, $0<\phi\in\mathscr{S}(\mathbb{R}^l\setminus\{0\})$ ($\mathscr{S}$ is the Schwartz space). A simple calculation yields

$$(\widehat{H}_p+1)\phi=X,\quad\phi(x)=0(|x|^k),$$
$$|\nabla\phi|=0(|x|^{k-1}),\quad(|x|\to 0).$$

Let η, ξ be elements of $C^\infty(\mathbb{R}^l)$ satisfying the conditions

$$\eta(x)=\begin{cases}1 & \text{if } |x|\geqslant\frac12,\\ 0 & \text{if } |x|\leqslant\frac14,\end{cases}\quad \xi(x)=\begin{cases}1 & \text{if } |x|\leqslant 1,\\ 0 & \text{if } |x|\geqslant 2.\end{cases}$$

Denote $\omega_n(x)=\eta(nx)\xi(x/n)$, $n=1,2,\ldots$, and $\phi_n=\omega_n\phi$. Then $0\leqslant\phi_n\in C_0^\infty(\mathbb{R}^l\setminus\{0\})$ and $\Delta\phi_n=\phi\Delta\omega_n+2\nabla\omega_n\nabla\phi+\omega_n\Delta\phi$. Thus

$$0\geqslant\int_{\mathbb{R}^l}|h|(-\Delta-[\beta(p)/|x|^2]+1)\phi_n(x)\,dx$$
$$=\langle|h|,\omega_nX\rangle-\langle|h|,\phi\Delta\omega_n\rangle-2\langle|h|,\nabla\phi\nabla\omega_n\rangle.$$

It is easy to see that

$$\langle|h|,\omega_nX\rangle\to\langle|h|,X\rangle,$$
$$\langle|h|,\phi\Delta\omega_n\rangle\to 0,\qquad(5.1)$$
$$\langle|h|,\nabla\phi\nabla\omega_n\rangle\to 0.$$

Hence $\langle|h|,X\rangle\leqslant 0$, so $h\equiv 0$. Thus (a) is proved.

(b) $p>2l/(l+2)$, there is $q_p\in(2l/(l+2))$ such that $\beta(q_p)>\beta(p)$ (see Fig. 1). It follows from Theorem 5.1 that $\exp(-tH_{qp})$ is a quasi-bounded C_0-semigroup in L^{q_p} and, consequently, $\epsilon(t)\equiv[\exp(-tH_{qp})\upharpoonright L^{q_p}\cap L^p]^\sim$ is a quasi-bounded C_0-semigroup in L^p. Denote the generator of $\epsilon(t)$ by C_p. Then $C_p\supset\widehat{H}_p$ (see Theorem 4.2). The latter and (a) give $C_p=H_p$.

Finally (c) follows from (a) and the Lumer–Phillips theorem[25].

Remarks: (1) In the case $p=2$ Theorem 5.2 was first proved by B. Simon[27] (see also Ref. 24). The idea of Simon's proof consists in the construction of the function $\phi_0>0$ with a certain asymptotic in $|x|\to 0$, which is the solution (in some sense) of the equality $(-\Delta-[\beta(2)/|x|^2]+1)\phi_0=0$. The above given proof of part (a) Theorem 5.2 is close to the Kalf–Walter method.[28]

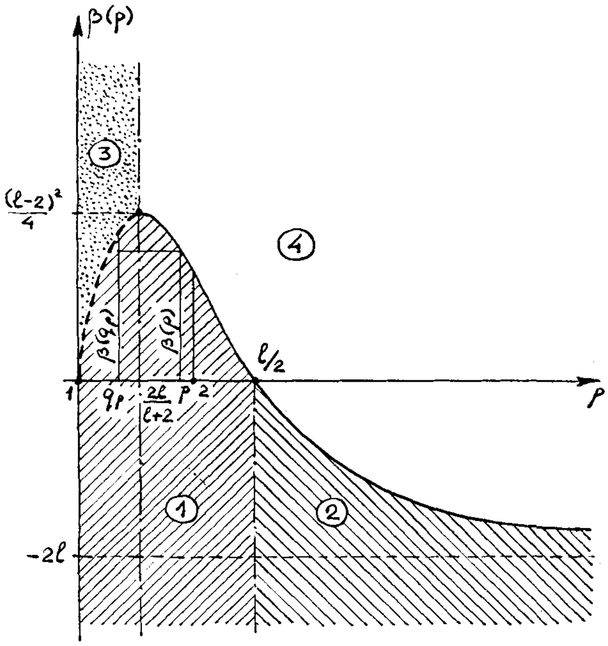

FIG. 1. (1) H_p is a generator of the quasi-bounded holomorphic semigroup in L^p; (2) H_p is a generator of the contraction semigroup in L^p; (3) All $\lambda < 0$ are eigenvalues of the operator $\widehat{H}_p$; (4) $\mathrm{Ran}(\widehat{H}_p + 1)$ is not dense in L^p for any $\lambda > 0$.

(2) Let us explain the method of construction of the functions ϕ, X. They must obey the following requirements: $0 < X \in L^p$, $0 < \phi \in \mathscr{S}(\mathbb{R}^l \setminus \{0\})$, $(\widehat{H}_p + 1)\phi = X$. For the validity of the relations (5.1) a certain asymptotic behavior of ϕ, X is necessary. However, to obtain the optimal result, it is also necessary $|x|^{-2}\phi \in L^p_w$.

(3) The constant $\beta(p)$ in Theorem 5.2 is optimal. In fact, consider the operator $\widehat{H}_p = (-\Delta - (\beta/|x|^2) + \lambda) \upharpoonright \mathscr{S}(\mathbb{R}^l \setminus \{0\}), \lambda > 0, \beta > \beta(p)$ and the function $h(x) = |x|^{-(l-2)/2} K_\nu \sqrt{(\lambda}\, |x|)$, $\nu = \frac{1}{2}\sqrt{|(l-2)^2 - 4\beta}$, where K_ν is a modified Bessel function (see Ref. 29). Let $p \leqslant 2l/(l+2)$, then it is not difficult to see that $h \in L^p$ and $\widehat{H}_p h = 0$. If $p > 2l/(l+2)$, then $h \in L^{p'}$. Since $-\Delta u \in C_0^\infty(\mathbb{R}^l \setminus \{0\})$, $|x|^{-2} u \in C_0^\infty(\mathbb{R}^l \setminus \{0\})$ for any $u \in C_0^\infty(\mathbb{R}^l \setminus \{0\})$ and $D = \langle u, (-\Delta - \beta |x|^{-2} + \lambda) h \rangle = \langle (-\Delta - \beta |x|^{-2} + \lambda) u, h \rangle$, so $\mathrm{Ran}(\widehat{H}_p + 1)$ is not dense in L^p. Thus we can represent all the results obained in Theorem 5.2 in the following way (see Fig. 1).

(4) The condition $\beta \leqslant \beta(p)$ for the operator $(-\Delta(\beta/|x|^2)) \upharpoonright C_0^\infty(\mathbb{R}^l \setminus \{0\})$, when $1 < p < l/2$ was obtained by two different methods. This assumption follows from the condition $V \in P_p$ in Theorem 5.1 and it is the consequence of the Kalf–Walter method in Theorem 5.2.

Finally we shall prove an inequality which is very useful in the spectral theory of the Schrödinger operator.

Lemma 5.3 (*generalized Schmincke inequality*): Let $l \geqslant 3$ and $\epsilon > 0$. Then for any $1 < p < l/2$

$$\left\| \left(-\Delta - \frac{\beta(p) - \epsilon}{|x|^2} + 1 \right) u \right\|_p \geqslant \frac{1}{\epsilon} \left\| \frac{1}{|x|^2} u \right\|_p. \quad (5.2)$$

Proof: The above results imply that (5.2) is equivalent to

$$\left\| \frac{1}{|x|^2} \left(-\Delta - \frac{\beta(p) - \epsilon}{|x|^2} + 1 \right)^{-1} \right\|_{p,p} \leqslant \frac{1}{\epsilon}. \quad (5.3)$$

Using C. Neumann series, we obtain

$$\left\| \frac{1}{|x|^2} \left(-\Delta - \frac{\beta(p) - \epsilon}{|x|^2} + 1 \right)^{-1} \right\|_{p,p} = \frac{1}{\beta(p) - \epsilon} \times \left\| \sum_{m=0}^{\infty} (-1)^m \left[\frac{\beta(p) - \epsilon}{|x|^2} (-\Delta + 1)^{-1} \right]^{m+1} \right\|_{p,p} \leqslant \frac{1}{\beta(p) - \epsilon} \sum_{m=0}^{\infty} \left\| \frac{\beta(p) - \epsilon}{|x|^2} (-\Delta + 1)^{-1} \right\|_{p,p}^{m+1}.$$

Thus Corollary 2.9 and direct computations give (5.3). ■

6. EXACT L^p ESTIMATES OF EIGENFUNCTIONS AND GENERALIZED EIGENFUNCTIONS OF THE SCHRÖDINGER OPERATOR

The main results of this section is

Theorem 6.1: Let $l \geqslant 3$, $V = V^+ - V^-$, $V^\pm \geqslant 0$, $0 \leqslant \beta < ((l-2)/2)^2$, Suppose that

(1) $V^+ \in L^1_{\mathrm{loc}}(\mathbb{R}^l \setminus S)$, where S is a closed set of Lebesque measure zero;

(2) $V^- \in L^{l/2}_w(\mathbb{R}^l)$ and $\|V^-\|_{l/2,w} \leqslant \Omega_l^{2/l} \beta$. Let $H = H_0 \dotplus V$ is the form sum. Put

$$p'(\beta) = \frac{2l}{l - 2 - \sqrt{(l-2)^2 - 4\beta}},$$

$$\frac{1}{p(\beta)} + \frac{1}{p'(\beta)} = 1.$$

Then (a) $\|(H + \lambda)^{-N} u\|_q \leqslant \mathrm{const}\|u\|_\nu$ for all sufficiently large $\lambda > 0$ and convenient $N \geqslant 1$; (b) $\|\exp\|(-tH)u\|_q \leqslant \mathrm{const}\|u\|_\nu$, where $\nu \in (p(\beta), p'(\beta))$, $q \in [\nu, p'(\beta))$, $u \in L^q \cap L^\nu \cap L^2$.

Before the proof of Theorem 6.1 we give some representations for $(H + \lambda)^{-1}$.

For $V \in PK$ the following representations are well known (see Ref. 22)

$$g = g_0 - g_0 |V|^{1/2} (1 + V^{1/2} g_0 |V|^{1/2})^{-1} V^{1/2} g_0, \quad (6.1)$$

$$g = g_0^{1/2} (1 + g_0^{1/2} V g L_0^{1/2})^{-1} g_0^{1/2}, \quad (6.2)$$

where $g \equiv (H + \lambda)^{-1}$, $g_0 \equiv (H_0 + \lambda)^{-1}$ and $\lambda > 0$ is sufficiently large. And (6.1), (6.2) are understood in the $\mathscr{L}(L^2)$ sense.

Our purpose is to prove representations for $(H + \lambda)^{-1}$, when $V \in P_p$.

So let $V \in P_p$. Since $P_p \subset PK$, the form sum $H = H_0 \dotplus V$ is well defined. Consider the semigroup $\epsilon(t) = (\exp(-tH) \upharpoonright L^2 \cap L^q)^\sim$ in L^q space, where $q \in [\min\{p, p'\}, \max\{p, p'\}]$. We denote a generator of this semigroup by H_q; It is clear that the construction of H_q implies $(H_q + 1\lambda)^{-1} \upharpoonright L^2 \cap L^q = (H + \lambda)^{-1} \upharpoonright L^2 \cap L^q$.

Proposition 6.2: Let $1 < p < \infty$, $V \in P_p$ and $H_q = (H_0 \dotplus V)_q$, $q \in [\min\{p, p'\}, \max\{p, p'\}]$. Then

$$(Hp_s + \lambda)^{-1} = g_0 - g_0 |V|^{1-s} (1 + V^s g_0 |V|^{1-s})^{-1} V^s g_0 \quad (6.3)$$

(the quality in $\mathscr{L}(L^{p_s})$, where $0 < s \leqslant 1$, $1/p_s = 1 - s + (2s - 1)/p$, and $\lambda > 0$ is sufficiently large.

Proof: Using arguments analogous to the proof of Proposition 1.1 we can show

$V^s g_0 \in \mathcal{L}(L^{p_s}), \quad g_0 |V|^{1-s} \in \mathcal{L}(L^{p_s})$

(to see this, choose the family $T(z) = V^z g_0$ instead of $F(z) = V^z g_0 V^{1-z}$). Moreover, the definition of P_p and Proposition 1.1 imply

$$\| V^s g_0 |V|^{1-s} \|_{p_s p_s} < 1$$

for all sufficiently large $\lambda > 0$. Hence, the operator

$$g_s \equiv g_0 - g_0 |V|^{1-s} (1 + V^s g_0 |V|^{1-s})^{-1} V^s g_0$$

is correctly defined and $g_s \in \mathcal{L}(L^{p_s})$.

Define the operators

$$\Pi_n = g_0 + \sum_{k=1}^{n} (-1)^k (g_0 V q_0)^k, \quad n = 1,2,\cdots.$$

It is clear that $\Pi_n \in \mathcal{L}(L^{p_s})$, $n = 1,2,\cdots$, $s \in [0,1]$.

Let $f \in L^2 \cap L^{p_s}$, $0 < s \leqslant 1$, then, obviously,

$$\Pi_n f = g_0 f + \sum_{k=1}^{n} (-1)^k (g_0 |V|^{1-s} V^s g_0)^k f \xrightarrow[L^{p_s}]{s} g_s f \quad (n \to \infty).$$

It follows from (6.1) that $g_{1/2} = (H + \lambda)^{-1}$, so

$$g_s \restriction L^2 \cap L^{p_s} = (H + \lambda)^{-1} \restriction L^2 \cap L^{p_s} = (H_{p_s} + \lambda)^{-1} \restriction L^2 \cap L^{p_s}.$$

As $g_s \in \mathcal{L}(L^{p_s})$, $(H_{p_s} + \lambda)^{-1} \in \mathcal{L}(L^{p_s})$, and $L^2 \cap L^{p_s}$ is dense in L^p if $0 < s \leqslant 1$, so $g_s = (H_{p_s} + \lambda)^{-1}$. ■

Remark: In Proposition 6.2 we assume $s \neq 0$, because $p = 1$ and $s = 0$ imply $p_s = \infty$, and in this case $L^2 \cap L^{p_s}$ is not dense in L^{p_s} and we cannot write $g_s = (H_{p_s} + \lambda)^{-1}$. But if we know $p \neq 1$ *a priori*, we may put $s \in [0,1]$.

Proposition 6.3: Let $l \geqslant 3$, $V \in L^{l/2}_w$, $\|V\|_{l/2,w} \leqslant \Omega_l^{2/l} \beta$, $0 \leqslant \beta < ((l-2)/2)^2$. Suppose that $H = H_0 \dotplus V$ is the form sum and $p(\beta)$, $p'(\beta)$ are defined in Theorem 6.1. Then

$$(H + \lambda)^{-1} u = g_0^s B g_0^{1-s} \text{ (pointwise a.e)}$$

for $\forall u \in L^1 \cap L^\infty$ and all $\lambda > 0$, where $B \in \mathcal{L}(L^{p_s})$,

$$1/p_s = 1 - s + (2s-1)/p, \quad 0 < s < 1.$$

Proof. It is a direct consequence of Propositions 3.1 and 6.2. ■

Remark: A direct calculation shows that $B = (1 + g_0^{1-s} V g_0^s)^{-1}$ so that

$$(H + \lambda)^{-1} u = g_0^s (1 + g_0^{1-s} V g_0^s)^{-1} g_0^{1-s} u. \tag{6.4}$$

Proof of Theorem 6.1: Suppose at first $V^+ = 0$. Let $u \in L^1 \cap L^\infty$, $v \in (p(\beta), p'(\beta))$ and $q \in [v, p'(\beta))$, then it is clear that

$$\|(H + \lambda)^{-1} u\|_q = \|g_0^s B g_0^{1-s} u\|_q \leqslant \text{const} \|u\|_{q_1},$$

where $1/q = (1/q_1) + (1/k_1) - 1$, $1/k_1 > 1 - (2/l)$.

Using the reduction we have

$$\|(H + \lambda)^{-N} u\|_q \leqslant \text{const} \|u\|_{q_N},$$

where

$$1/q = (1/q_N) + \sum_{j=1}^{N} (1/k_j - 1), \; 1/k_j > 1 - \frac{2}{l}.$$

Choose N such that $q_N = v$. Then

$$\|(H + \lambda)^{-N} u\|_q \leqslant \text{const} \|u\|_v \quad \text{for suitable } N \geqslant 1. \tag{6.5}$$

Notice that e^{-tH} is consequently a holomorphic semigroup by Theorem 5.1.

$$\|e^{-tH} u\|_q = \|(H + \lambda)^{-N} (H + \lambda)^N e^{-tH} u\|_q \leqslant \text{const} \|(H + \lambda)^N e^{-tH}\|_{v,v} \|u\|_v < \infty.$$

Thus Theorem 6.1 is proved for the case $V^+ = 0$. As (see, for example, Ref. 26)

$|e^{-t(H_0 \dotplus (V^+ - V^-))} u| \leqslant e^{-t(H_0 \dotplus (-V^-))} |u|$ (pointwise a.e.),

so

$$\|e^{-t(H_0 \dotplus V)} u\|_q \leqslant \|e^{-t(H_0 \dotplus (-V^-))} |u|\|_q. \quad ■$$

Remark: Evidently, valid is the

Conjecture: Let $V \in PK$ and the $H_0^{1/2}$-bound of the operator $|V|^{1/2}$ equals $\beta^{1/2}$ for some $0 < \beta < 1$. Then

$$\|e^{-tH} u\|_q \leqslant \text{const} \|u\|_v, \quad \forall u \in L^2 \cap L^q \cap L^v,$$
$$n \in (t(\beta), t'(\beta)), \quad q \in [v, t'(\beta)),$$

where

$$t'(\beta) = \frac{2l}{(l-2)(1 - \sqrt{1-\beta})}, \; \frac{1}{t(\beta)} + \frac{1}{t'(\beta)} = 1.$$

This conjecture was proved in Theorem 6.1 for the case $V \in L^{l/2}_w(\mathbb{R}^l)$. Notice that I. Herbst and A. Sloan[30] proved the result analogous to our conjecture with $t'(\beta) = 2l/(l-2)\beta$.

Theorem 6.1 implies eigenfunction estimates for the operator H.

Corollary 6.4: Let ψ be an eigenfunction of the operator H. Then $\psi \in \bigcap_{2 \leqslant q < p'(\beta)} L^q$.

Proof: If $H\psi = \lambda\psi$, then $e^{-tH}\psi = e^{-\lambda t}\psi$. Thus putting $v = 2$ and using Theorem 6.1 we obtain

$$\|e^{-tH}\psi\|_q = e^{-\lambda t} \|\psi\|_q \leqslant \text{const} \|\psi\|_2 < \infty, \quad q \in [2, p'(\beta)). \quad ■$$

Corollary 6.4 is exact. In fact, consider the operator $H = H_0 \dotplus V$ in $L^2(\mathbb{R}^3)$ (for simplicity we discuss the case $l = 3$). Suppose that $V(x) = -\beta |x|^{-2}$, $\beta < \frac{1}{4}$ for $|x| < 1$, and a behavior of $V(x)$ on the set $|x| \geqslant 1$ is such that the operator H has an eigenfunction (which is sufficiently simple to construct such a V). It is known that the angular momentum zero eigenstates behave like $|x|^{-s}$, $s = \frac{1}{2}[1 - \sqrt{(1 - 4\beta)}]$ in the neighborhood of the origin (see Ref. 31, Sec. 35). All other eigenstates vanish at the origin. Thus all the eigenstates of H are in L^p for $p < p'(\beta) = 6[1 - \sqrt{(1 - 4\beta)}]$.

Theorem 6.1 is an essential generalization of the Herbst–Sloan result in the case $V \in L^{l/2}_w$.

Consider now the operator $\rho^\delta (H + \lambda)^{\cdot} \rho^{-\delta}$, where $\rho(x) = (1 + |x|)$, $\delta \in \mathbb{R}'$. Our purpose is to get a result analogous to Theorem 6.1 for this operator.

We shall need the following

Lemma 6.5 [23]: Let $K_s(x,y,\lambda)$, $\lambda > 0$ be an integral kernel of the operator $(H_0 + \lambda)^{-s}$, $s > 0$. Suppose that $\delta \in \mathbb{R}^1$ and $x > 0$ are fixed. Then

$$\rho^\delta(x) K_s(x,y,\lambda) \rho^{-\delta}(y) \leqslant c(\theta,\lambda) K_s(x,y,\theta\lambda), \quad \theta \in (0,1). \tag{6.6}$$

Moreover, for any $\epsilon > 0$ there exsit $\theta_0(0,1)$, $\lambda = \lambda_0(\theta_0)$ such that $c(\theta_0,\lambda) \leqslant 1 + \epsilon$ for $\lambda \geqslant \lambda_0$.

Next, the following representations are valid in (see Ref. 23)

$$\rho^\delta(H_0 + V+\lambda)^{-1}\rho^{-\delta} = \rho^\delta(H_0+\lambda)^{-1}\rho^{-\delta} \times [1 + V\rho^\delta(H_0+\lambda)^{-1}\rho^{-\delta}]^{-1}, \quad V\in P_2,$$

$$\rho^\delta(H_0 \dot{+} V+\lambda)^{-1}\rho^{-\delta} = \rho^\delta(H_0+\lambda)^{1/2}\rho^{-\delta} \times [1+\rho^\delta(H_0+\lambda)^{-1/2}V(H_0+\lambda)^{-1/2}\rho^{-\delta}]^{-1} \times\rho^\delta(H_0+\lambda)^{-1/2}\rho^{-\delta}, \quad V\in PK.$$

for all sufficiently large $\lambda > 0$.

But analogous arguments and Proposition 6.2 give the following representation [in the $\mathscr{L}(L^p)$ sense]

$$\rho^\delta(H_{\dot{p}_s} + \lambda)^{-1}\rho^{-\delta} = \rho^\delta(H_0+\lambda)^{-s}\rho^{-\delta} \times [1+\rho^\delta(H_0+\lambda)^{-1+s}V(H_0+\lambda)^{-s}\rho^{-\delta}]^{-1} \times\rho^\delta(H_0+\lambda)^{-1+s}\rho^{-\delta},$$

where

$$V\in P_p,\ 1/p_s = 1-s+(2s-1)/p,\ s\in(0,1).$$

Now it is clear that (6.5), (6.6), and arguments analogous to the proof of Theorem 6.1 imply

Theorem 6.6: Suppose that all the assumptions of Theorem 6.1 are valid. Let $\rho(x) = (1+|x|)$, $\delta\in\mathbb{R}^1$. Then

$$\|\rho^\delta(H+\lambda)^{-N}\rho^{-\delta}u\|_q \leqslant \text{const}\|u\|_v, \quad \forall u\in L^q\cap L^v\cap L^2$$

for all sufficiently large $\lambda > 0$ and suitable $N\geqslant 1$, where

$$v\in(\rho(\beta),p'(\beta)), \quad q\in[v,p'(\beta)).$$

Let us consider now some properties of generalized eigenfunctions of the operator $H = H_0 \dot{+} V$. There is a complete discussion of the eigenfunction expansion theory in Berezanskiĭ.[32] So we shall give only some main results of this theory which was obtained for the operator H in Ref. 23 (see also Refs. 33 and 34 for the case $l = 3$).

Let $V = V^+ - V^-$, $0\leqslant V^+\in L^1_{\text{loc}}(\mathbb{R}^l\setminus S)$, $0\leqslant V^-\in PK$, where S is a closed set of Lebesque measure zero. Let $H = H_0 \dot{+} V$ is the form sum in the $\mathscr{H}_0\equiv L^2$. Introduce the notation $L^2_\delta = L^2(\mathbb{R}^l,\rho^\delta(x)\,dx)$ and consider the scale

$$Д\subset\mathscr{H}_+\subset\mathscr{H}_0\subset\mathscr{H}_-\subset Д', \tag{6.7}$$

where

$$\delta>0,\ \mathscr{H}_+ = L^2_\delta,\ \mathscr{H}_- = L^2_{-\delta},$$

$$Д = \{\varphi : \varphi\in\mathscr{D}(H)\cap L^2_\delta,\ H_\varphi\in L^2_\delta\}$$

and $Д'$ is a corresponding antidual space (see Ref. 32).

Recently, V. F. Kovalenko and Yu. A. Semenov[23] have proved that the scale (6.7) with $\delta > l$ may be used for the eigenfunction expansion of the operator H. Namely, they examined the conditions:

(1) $\rho^{-\delta}e^{-tH}$ is the Hilbert-Schmidt operator;

(2) $Д$ is dense in $\mathscr{H}_+$;

(3) H is a continuous map from $Д$ in $\mathscr{H}^+$.

Following Berezanskii,[32] we call function $\psi\in\mathscr{H}_-$ a generalized eigenfunction of the operator H, if

$$\langle\psi,H_\varphi\rangle = E\langle\psi,\varphi\rangle \text{ or } \langle\psi,(H+\lambda)\varphi\rangle = (E+\lambda)\langle\psi,\varphi\rangle,\ \lambda>0$$

for any $\varphi\in Д$.

Using a concrete form of the scale (6.7) we may put $\varphi\,(H+\lambda)^{-1}g$, where $g\in L^2_\delta$. Notice that Lemma 6.6 implies $(H+\lambda)^{-1}\in\mathscr{L}(L^2_\delta)$, so that $\varphi\in Д$ in fact. Then

$$\langle\psi,g\rangle = (E+\lambda)\langle\psi,(H+\lambda)^{-1}g\rangle$$

and

$$\langle\rho^{-\delta/2}\psi,\rho^{\delta/2}g\rangle = (E+\lambda)\langle\rho^{-\delta/2}\psi,\rho^{\delta/2}(H+\lambda)^{-1}\rho^{-\delta/2}\rho^{\delta/2}g\rangle. \tag{6.8}$$

As g is an arbitrary element of L^2_δ, (6.8) implies

$$\rho^{-\delta/2}\psi = (E+\lambda)\rho^{-\delta/2}(H+\lambda)^{-1}\rho^{\delta/2}\rho^{-\delta/2}\psi$$

and, moreover,

$$\rho^{-\delta/2}\psi = (E+\lambda)^m\rho^{-\delta/2}(H+\lambda)^{-m}\rho^{\delta/2}\rho^{-\delta/2}\psi \tag{6.9}$$

Since Lemma 6.5 and Theorem 6.1 yield $\rho^{-\delta/2}(H+\lambda)^{-m}\rho^{\delta/2}\in\mathscr{L}(L^2,L^p)$ with $p\in[2,p'(\beta))$ and suitable $m>0$, (6.9) implies the estimate

$$\|\rho^{-\delta/2}\psi\|_q \leqslant \text{const}\|\rho^{-\delta/2}\psi\|_2 = \text{const}\|\psi\|_{\mathscr{H}_-} < \infty. \tag{6.10}$$

Thus we proved

Theorem 6.7: Suppose that all the assumptions of Theorem 6.1 are valid. Then all generalized eigenfunctions of the operator H obey the condition

$$\rho^{-\delta/2}\psi\in L^q$$

for any $q\in[2,p'(\beta))$ and $\delta > l$.

Remark: Let $V^-\in L^{l/2}_w$. As we noted, $V^-\in P_l$ is invalid. Thus Theorem 6.7 does not give any information in the case $V^-\in P_1$. But this problem was completely investigated in Ref. 23. In particular, it was proved that it is possible to put $q=\infty$ in (6.10) so that we have pointwise estimates of the generalized eigenfunctions: $\psi(x)\leqslant\text{const}\rho^{\delta/2}(x)$, $\forall\delta>l$.

Finally, we consider the sequilinear form $\Sigma^l_{k=1}\langle(i(\partial/\partial x_k)+a_k)u,(i(\partial/\partial x_k)+a_k)u\rangle$, where a_k is a real valued function from $L^2_{\text{loc}}(\mathbb{R}^k\setminus S)$, S is a closed set of Lebesque measure zero. Denote an operator associated with the closure of this form by $H(\mathbf{a})$. It was noted by E. Nelson that the Feynman–Kac–Ito formula implies $|\exp(-tH(\mathbf{a}))u|\leqslant\exp(-tH_0)|u|$ a.e. (see, for example, Ref. 35). So many of our results may be extended to the operator $H = H(\mathbf{a}) \dot{+} V$.

Note added in proof (by B. Simon): The conjecture at the end of Sec. 3 is false. If T is a linear map from R^l to R and $g\in L^1(R)$, then $V(x) = g(Tx)$ is in PK but may not be in the conjectured local weak L^p space.

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Variable-phase approach to off-shell scattering by nonlocal potentials

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The basic ideas of the variable-phase approach are used to develop first-order differential equations for the quasiphase parameters which describe the half-off-shell scattering amplitudes for a nonlocal potential. The on-shell equation of Calogero and Sobel's equation for a local potential are obtained as special cases.

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Pioneered by Morse and Allis,[1] the variable-phase approach (VPA) to potential scattering has been beautifully expounded by Calogero, Babikov and others.[2] In this approach the phase shifts are obtained as limiting values of certain phase functions, which are calculated by solving-first order differential equations. To describe the half-off-shell scattering amplitudes for a local potential Sobel[3] introduced the concept of the quasiphase parameter and wrote a first-order differential equation for this quasiphase parameter. Dolinszky[4] made an attempt to derive first-order linear differential equations for the completely off-shell phase shift in terms of the cut-off radius of the local two-body interaction. In a recent paper[5] we pointed out that his approach is defective, and constructed an equation for the fully off-shell scattering amplitude by employing one of the results derived by Tikochinsky.[6] In this work we use the variable-phase approach to derive a differential equation for the quasiphase parameter which relates the half-off-shell scattering amplitudes for a nonlocal potential. We use throughout this paper a system of units in which $\hbar = 2m = 1$.

A cut-off nonlocal potential $V_l^y(r,s)$ having the cut-off parameter y is defined as

$$V_l^y(r,s) = V_l(r,s), \quad r<y, \qquad V_l^y(r,s) = 0, \quad r\geqslant y, \tag{1}$$

where

$$V_l(r,s) = 2\pi rs \int_{-1}^{+1} d(\cos\theta)\, P_l(\cos\theta) V(\mathbf{r},\mathbf{s}). \tag{2}$$

For such a potential, the l-wave half-off-shell T matrix may be written as

$$T_l(k,q,k^2,y) = \frac{2}{\pi kq} \exp[i\delta_l^y(k)] \int_0^y \hat{j}_l(qr)\, dr \times \int_0^\infty V_l(r\,s) v_l^y(s)\, ds, \tag{3}$$

which can be expressed in terms of the so-called quasiphase function $\Delta_l(k,q,y)$ as

$$T_l(k,q,k^2,y) = -\frac{2}{\pi k} \exp[i\delta_l^y(k)] \Delta_l(k,q,y). \tag{4}$$

From Eqs. (3) and (4), we have

$$\Delta_l(k,q,y) = -\frac{1}{q} \int_0^y \hat{j}_l(qr)\, dr \int_0^\infty V_l(r,s) v_l^y(s)\, ds. \tag{5}$$

For the on-shell case, $q \rightarrow k$, Eq. (4) becomes

$$T_l(k,k,k^2,y) \equiv T_l(k,y) = -\frac{2}{\pi k} \exp[i\delta_l^y(k)] \sin\delta_l^y(k). \tag{6}$$

The wavefunction v_l^y used in Eq. (3) satisfies the differential equation

$$\left[\frac{d^2}{dr^2} + k^2 - \frac{l(l+1)}{r^2}\right] v_l^y(r) = \int_0^\infty V_l^y(r,s) v_l^y(s)\, ds, \tag{7}$$

and is specified by the boundary condition

$$[v_l^y(r)]_{r=0} = 0, \tag{8a}$$

$$v_l^y(r) \underset{r\rightarrow\infty}{\longrightarrow} \sin[kr - l\pi/2 + \delta_l^y(k)]. \tag{8b}$$

Here $\delta_l^y(k)$ is the phase shift induced by the cut-off potential $V_l^y(r,s)$.

The variable-phase approach proceeds by introducing the phase function $\delta_l^y(r)$ and amplitude function $\alpha_l^y(r)$ through a pair of equations:

$$v_l^y(r) = \alpha_l^y(r)\{\cos\delta_l^y(r)\hat{j}_l(kr) - \sin\delta_l^y(r)\hat{\eta}_l(kr)\}, \tag{9}$$

$$\frac{dv_l^y(r)}{dr} = k\alpha_l^y(r)\{\cos\delta_l^y(r)\hat{j}_l'(kr) - \sin\delta_l^y(r)\hat{\eta}_l'(kr)\}. \tag{10}$$

Here prime denotes differentiation with respect to the argument. Within the interval $r = (0,y)$ we may drop the superscript y on $\delta_l^y(r)$ because $\delta_l(r)$ may then be interpreted as the phase shift due to the potential $V_l^r(r',s)$, obtained by cutting off the potential $V_l(r',s)$ at $r' = r$. Thus $\delta_l(r)$ is independent of the cut-off parameter y insider this cut-off point i.e.,

$$\delta_l^y(r) = \delta_l(r), \quad r\leqslant y. \tag{11}$$

Comparing the first derivative of Eq. (9) with Eq. (10), we obtain

$$\delta_l^y(r) = \exp\left[-\int_r^y \left(\frac{\sin\delta_l(t)\hat{j}_l(kt) + \cos\delta_l(t)\hat{\eta}_l(kt)}{\cos\delta_l(t)\hat{j}_l(kt) - \sin\delta_l(t)\hat{\eta}_l(kt)}\right)\delta_l'(t)\, dt\right], \quad r\leqslant y. \tag{12}$$

The upper limit of the integral in Eq. (12) corresponds to a constant of integration which is consistent with the asymptotic boundary condition set up by Eq. (8b). At the cut-off point $r = y$

$$[\alpha_l^y(r)]_{r=y} = 1. \tag{13}$$

Equation (12) implies the differential equation

$$\frac{d\alpha_l^y(r)}{dy}$$

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$$= -\left[\frac{\sin\delta_l(y)\hat{j}_l(ky) + \cos\delta_l(y)\hat{\eta}_l(ky)}{\cos\delta_l(y)\hat{j}_l(ky) - \sin\delta_l(y)\hat{\eta}_l(ky)}\right]\delta_l'(y)\alpha_l^y(r). \quad (14)$$

The differential equation for the phase function may be obtained by differentiating Eq. (10) and then using the Schrödinger equation (7). We thus have

$$\delta_l'(y) = -\frac{1}{k}[\cos\delta_l(y)\hat{j}_l(ky) - \sin\delta_l(y)\hat{\eta}_l(ky)]^2 \times \int_0^\infty V_l(y,s)\frac{v_l^y(s)}{v_l^y(y)}\,ds. \quad (15)$$

Equations (9) and (10) can be used to write the ratio $v_l^y(s)/v_l^y(y)$ in the form

$$\frac{v_l^y(s)}{v_l^y(y)} = \exp\left[k\int_y^s\left(\frac{\cos\delta_l(p)\hat{j}_l'(kp) - \sin\delta_l(p)\hat{\eta}_l'(kp)}{\cos\delta_l(p)\hat{j}_l(kp) - \sin\delta_l(p)\hat{\eta}_l(kp)}\right)dp\right]. \quad (16)$$

Substituting Eq. (16) in Eq. (15), we get

$$\delta_l'(y) = -\frac{1}{k}[\cos\delta_l(y)\hat{j}_l(ky) - \sin\delta_l(y)\hat{\eta}_l(ky)]^2\int_0^\infty V_l(y,s)\,ds\exp\left[k\int_y^s\left(\frac{\cos\delta_l(p)\hat{j}_l'(kp) - \sin\delta_l(p)\hat{\eta}_l'(kp)}{\cos\delta_l(p)\hat{j}_l(kp) - \sin\delta_l(p)\hat{\eta}_l(kp)}\right)dp\right], \quad (17)$$

which is the well-known phase equation of Calogero.[7]

Let us now proceed to derive the differential equation for the quasiphase function $\Delta_l(k,q,y)$. To do this we differentiate Eq. (5) with due respect to the appearance of the cut-off radius y both in the integrand and in the upper limit of the integration. We thus obtain

$$\frac{d\Delta_l(k,q,y)}{dy} = -\frac{1}{q}\hat{j}_l(qy)\int_0^\infty V_l(y,s)v_l^y(s)\,ds - \frac{1}{q}\int_0^y \hat{j}_l(qr)\,dr\int_0^\infty V_l(r,s)\frac{dv_l^y(s)}{dy}\,ds. \quad (18)$$

The derivative $dv_l^y(s)/dy$ in Eq. (18) may be expressed in terms of $v_l^y(s)$ and $\delta_l'(y)$ with the help of Eqs. (9) and (14). Then using Eqs. (5), (16) and (17), we get

$$\begin{aligned}\frac{d\Delta_l(k,q,y)}{dy} &= -[\cos\delta_l(y)\hat{j}_l(ky) - \sin\delta_l(y)\hat{\eta}_l(ky)]\\ &\times\left[\frac{1}{q}\hat{j}_l(qy) - \frac{1}{k}\Delta_l(k,q,y)\{\sin\delta_l(y)\hat{j}_l(ky) + \cos\delta_l(y)\hat{\eta}_l(ky)\}\right]\\ &\times\int_0^\infty V_l(y,s)\,ds\exp\left[k\int_y^s\left(\frac{\cos\delta_l(p)\hat{j}_l'(kp) - \sin\delta_l(p)\hat{\eta}_l'(kp)}{\cos\delta_l(p)\hat{j}_l(kp) - \sin\delta_l(p)\hat{\eta}_l(kp)}\right)dp\right]. \quad (19)\end{aligned}$$

Equation (19) is the desired differential equation for the quasiphase function $\Delta_l(k,q,y)$. One may solve Eq. (19) simultaneously with Eq. (17) subject to the boundary conditions

$$\delta_l(0) = \Delta_l(k,q,0) = 0 \quad (20)$$

and $\Delta_l(k,q,\infty)$, the quasiphase for the full potential. The differential equation for the quasiphase function $\Delta_l(k,q,y)$ is coupled to the equation for the phase function $\delta_l(y)$ and has very complicated mathematical structure. To ensure the correctness of the results presented one can perform a couple of checks.

(i) For a local potential, Eq. (19) reduces to Sobel's equation for the quasiphase.[3]

(ii) In the limit $q\to k$, $\Delta_l(k,q,y)\to\sin\delta_l(y)$, Eq. (19) yields the corresponding on-shell result given by Eq. (17).

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Bound on the diffraction peak for the spin 0–spin 1/2 case

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We apply a recently developed method by the author to the problem of the diffraction peak bound for the spin 0–spin 1/2 particle scattering with the spin taken fully into account. The variational technique is used with the constraints, the total cross section, elastic cross section, and the unitarity of partial waves.

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I. INTRODUCTION

In a previous paper[1] we extended the variational method with inequality constraints[2] to arbitrary spin cases. The basic idea was to define a set of classes such that a set of partial wave amplitudes with the same l value belong to one and only one of those classes.

The method makes it possible to investigate the MacDowell, Martin[3] problem with the spin taken fully into account. Since also the unitarity of the partial waves is used in its full form, rather than as positiveness or boundedness, we can use the elastic cross section, rather than the contributions of the imaginary parts of the partial waves to the elastic cross section, as one of the constraints. The remaining constraints are the total cross section and the unitarity of the partial waves.

In Sec. II we write the equations for the constraints as well as for the forward slope. We form the Lagrange's function and differentiating it we obtain four equations in terms of Lagrange parameters. Taking second derivatives we find also the extremum conditions. In this section we also define the four classes determined by the unitarity equations.

In Sec. III the forms of the partial waves are determined in different classes using the unitarity and the extremum conditions. We also find conditions on Lagrange multipliers. The range of the partial waves is determined by the multipliers. Fitting the total and elastic cross sections, the multipliers are found which minimize the forward slope.

In Sec. IV we summerize and discuss our results.

II. FORMALISM

We define S, A_0, and E in terms of $dA/dt|_{t=0}$, σ^T, and σ^{El}

$$S = 4k^2 \frac{k}{\sqrt{s}} \left.\frac{dA}{dt}\right|_{t=0} = \sum l(l+1)[(l+1)a_{l+} + l a_{l-}], \quad (1)$$

$$A_0 = \frac{k^2}{4\pi}\sigma^T = \sum [(l+1)a_{l+} + l a_{l-}], \quad (2)$$

$$E = \frac{k^2}{4\pi}\sigma^{El} = \sum [(l+1)(a_{l+}{}^2 + r_{l+}{}^2) + l(a_{l-}{}^2 + r_{l-}{}^2)]. \quad (3)$$

Here k is the c.m. wavenumber, s is the c.m. total energy squared, $dA/dt|_{t=0}$ is the forward slope, σ^T is the total cross section, σ^{El} is the elastic cross section, and $a_{l+}, a_{l-}, r_{l+}, r_{l-}$ are the imaginary and real parts of the partial waves f_{l+} and f_{l-}.

We also have the inequality constraints of unitarity:

$$u_l \equiv a_{l+} - a_{l+}{}^2 - r_{l+}{}^2 \geqslant 0, \quad (4)$$

$$v_l \equiv a_{l-} - a_{l-}{}^2 - r_{l-}{}^2 \geqslant 0, \quad (5)$$

We want to minimize $dA/dt|_{t=0}$ subject to constraints (2)–(5). The auxiliary function of Lagrange is

$$L = S + \alpha A_0 + \beta E + \sum (l+1)\lambda_l(a_{l+} - a_{l+}{}^2 - r_{l+}{}^2) + \sum l\mu_l(a_{l-} - a_{l-}{}^2 - r_{l-}{}^2). \quad (6)$$

Here $\lambda_l \geqslant 0$, $\mu_l \geqslant 0$ from the theory of inequality constraints. The factors $(l+1)$ and l under the series are chosen arbitrarily by modifying the definitions of λ_l and μ_l in order to simplify the resulting formulas.

We now differentiate L with respect to a_{l+}, a_{l-}, r_{l+}, and r_{l-}.

$$\frac{\partial L}{\partial a_{l+}} = 0 \text{ gives } a_{l+}(\beta - \lambda_l) + \tfrac{1}{2}[l(l+1) + \alpha + \lambda_l] = 0, \quad (7)$$

$$\frac{\partial L}{\partial a_{l-}} = 0 \text{ gives } a_{l-}(\beta - \mu_l) + \tfrac{1}{2}[l(l+1) + \alpha + \mu_l] = 0, \quad (8)$$

$$\frac{\partial L}{\partial r_{l+}} = 0 \text{ gives } r_{l+}(\beta - \lambda_l) = 0, \quad (9)$$

$$\frac{\partial L}{\partial r_{l-}} = 0 \text{ gives } r_{l-}(\beta - \mu_l) = 0. \quad (10)$$

The second derivatives are

$$\frac{\partial^2 L}{\partial a_{l+}{}^2} = 2(l+1)(\beta - \lambda_l),$$

$$\frac{\partial^2 L}{\partial a_{l-}{}^2} = 2l(\beta - \mu_l),$$

$$\frac{\partial^2 L}{\partial r_{l+}{}^2} = 2(l+1)(\beta - \lambda_l),$$

$$\frac{\partial^2 L}{\partial r_l{}^2} = 2l(\beta - \mu_l).$$

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All other derivatives vanish. Minimum conditions are

$$\beta \geqslant \lambda_l, \quad \beta \geqslant \mu_l. \tag{11}$$

We now define the following four classes:

$$I^+I^- = \{l \,|\, \mu_l > 0, v_l > 0\}, \quad \lambda_l = 0, \quad \mu_l = 0, \tag{12}$$

$$I^+B^- = \{l \,|\, \mu_l > 0, v_l = 0\}, \quad \lambda_l = 0, \quad \mu_l \geqslant 0, \tag{13}$$

$$I^-B^+ = \{l \,|\, \mu_l = 0, v_l > 0\}, \quad \lambda_l \geqslant 0, \quad \mu_l = 0, \tag{14}$$

$$B^+B^- = \{l \,|\, \mu_l = 0, v_l = 0\}, \quad \lambda_l \geqslant 0, \quad \mu_l \geqslant 0. \tag{15}$$

A pair of partial wave amplitudes f_{l+}, f_{l-} with the same l value belongs to one and only one of these classes.

III. FOUR CLASSES AND PARTIAL WAVES

A. Class I^+I^-

In this class $\lambda_l = 0, \mu_l = 0$. Hence the general equations (7)–(10) take in this class the following forms:

$$a_{l+}\beta + \tfrac{1}{2}[l(l+1) + \alpha] = 0, \tag{16}$$

$$a_{l-}\beta + \tfrac{1}{2}[l(l+1) + \alpha] = 0, \tag{17}$$

$$r_{l+} = 0, \tag{18}$$

$$r_{l-} = 0. \tag{19}$$

It is seen that

$$a_{l+} = a_{l-} = -(1/2\beta)[l(l+1) + \alpha]. \tag{20}$$

With the minimum condition $\beta > 0$ and the unitarity of partial waves we have

$$0 \leqslant -[l(l+1) + \alpha]/2\beta \leqslant 1, \tag{21}$$

$$0 \leqslant -[l(l+1) + \alpha] \leqslant 2\beta, \tag{22}$$

$$l(l+1) + \alpha \leqslant 0,$$

$$l(l+1) + \alpha + 2\beta \geqslant 0. \tag{23}$$

B. Class I^+B^-

In this class $\lambda_l = 0, \mu_l \geqslant 0$, and $v_l = 0$. Equations (7)–(10) take in this class the following forms:

$$a_{l+}\beta + \tfrac{1}{2}[l(l+1) + \alpha] = 0, \tag{24}$$

$$a_{l-}(\beta - \mu_l) + \tfrac{1}{2}[l(l+1) + \alpha + \mu_l] = 0, \tag{25}$$

$$r_{l+} = 0, \tag{26}$$

$$r_{l-}(\beta - \mu_l) = 0. \tag{27}$$

Also

$$v_l \equiv a_{l-} - a_{l-}^{\,2} - r_{l-}^{\,2} = 0, \tag{28}$$

$$r_{l-} = 0 \text{ gives } a_{l-} = \begin{matrix}\nearrow 1 \\ \searrow 0\end{matrix}. \tag{29}$$

When $a_{l-} = 1$, Eq. (25) becomes

$$l(l+1) + \alpha + \mu_l = 2(\mu_l - \beta)$$

or

$$\mu_l = \alpha + 2\beta + l(l+1). \tag{30}$$

With the minimum condition (11) we have

$$\alpha + \beta + l(l+1) \leqslant 0. \tag{31}$$

When $a_{l-} = 0$, Eq. (25) becomes

$$\mu_l = -[l(l+1) + \alpha]. \tag{32}$$

The minimum condition (11) gives

$$\alpha + \beta + l(l+1) \geqslant 0. \tag{33}$$

C. Class I^-B^+

In this class $\mu_l = 0, \lambda_l \geqslant 0$, and $\mu_l = 0$. Equations (5)–(7) take the forms

$$a_{l-}\beta + \tfrac{1}{2}[l(l+1) + \alpha] = 0, \tag{34}$$

$$a_{l+}(\beta - \lambda_l) + \tfrac{1}{2}[l(l+1) + \alpha + \lambda_l] = 0, \tag{35}$$

$$r_{l-} = 0, \tag{36}$$

$$r_{l+}(\beta - \lambda_l) = 0. \tag{37}$$

Also

$$u_l \equiv a_{l+} - a_{l+}^{\,2} - r_{l+}^{\,2} = 0, \tag{38}$$

$$r_{l+} = 0 \text{ gives } a_{l+} = \begin{matrix}\nearrow 1 \\ \searrow 0\end{matrix}. \tag{39}$$

When $a_{l+} = 1$, Eq. (35) becomes

$$l(l+1) + \alpha + \lambda_l = 2(\lambda_l - \beta)$$

or

$$\lambda_l = l(l+1) + \alpha + 2\beta. \tag{40}$$

With the minimum condition (11) we have

$$\alpha + \beta + l(l+1) \leqslant 0. \tag{41}$$

When $a_{l+} = 0$, Eq. (35) becomes

$$\lambda_l = -[l(l+1) + \alpha]. \tag{42}$$

The minimum condition (11) gives

$$\alpha + \beta + l(l+1) \geqslant 0. \tag{43}$$

D. Class B^+B^-

In this class $u_l = 0, v_l = 0$. The forms of the equations in this class are

$$a_{l+}(\beta - \lambda_l) + \tfrac{1}{2}[l(l+1) + \alpha + \lambda_l] = 0,$$

$$a_{l-}(\beta - \mu_l) + \tfrac{1}{2}[l(l+1) + \alpha + \mu_l] = 0, \tag{44}$$

$$(\beta - \lambda_l) r_{l+} = 0, \quad (\beta - \mu_l) r_{l-} = 0, \tag{45}$$

$$a_{l+} - a_{l+}^{\,2} - r_{l+}^{\,2} = 0, \quad a_{l-} - a_{l-}^{\,2} - r_{l-}^{\,2} = 0, \tag{46}$$

$$r_{l+} = 0 \text{ gives } a_{l+} = \begin{matrix}\nearrow 1 \\ \searrow 0\end{matrix},$$

$$r_{l-} = 0 \text{ gives } a_{l-} = \begin{matrix}\nearrow 1 \\ \searrow 0\end{matrix}. \tag{47}$$

When $a_{l+} = 1$, Eq. (44) gives:

$$\lambda_l = \alpha + 2\beta + l(l+1).$$

When $a_{l-} = 1$, Eq. (44) gives:

$$\mu_l = \alpha + 2\beta + l(l+1) \cdot \tag{48}$$

The minimum conditions (11) give

$$\alpha + \beta + l(l+1) \leqslant 0 \tag{49}$$

For $a_{l+} = a_{l-} = 1$ we also have $\lambda_l = \mu_l$.

When $a_{l+} = 0$, Eq. (44) gives:

$$\lambda_l = -[l(l+1) + \alpha].$$

When $a_{l-} = 0$, Eq. (44) gives

$$\mu_l = -[l(l+1)+\alpha]. \quad (50)$$

The minimum conditions (11) give

$$\alpha+\beta+l(l+1)\geqslant 0. \quad (51)$$

We thus see that in all classes two possibilities exist:

$$\text{(A) either } (\alpha+\beta)+l(l+1)\leqslant 0, \quad (52)$$

$$\text{(B) or } (\alpha+\beta)+l(l+1)\geqslant 0, \quad (53)$$

except the class I^+I^- in which

$$(\alpha+\beta)+l(l+1)\geqslant -\beta. \quad (54)$$

For case (B) this is automatically satisfied. For case (A) it is satisfied between $-\beta$ and 0.

Let us now look at the expression $y=(\alpha+\beta)+l(l+1)$ as a function of l. This represents a paralola with its extremum at $l=-\frac{1}{2}$. This extremum is always a minimum, where the value of the function is

$$y=(\alpha+\beta)-\tfrac{1}{4}.$$

Hence $(\alpha+\beta)+l(l+1)\geqslant 0$, if $(\alpha+\beta)\geqslant\frac{1}{4}$, and this for all values of l. If $\alpha+\beta<\frac{1}{4}$ then $(\alpha+\beta)+l(l+1)\leqslant 0$ for a limited range of l. This range is between $l=-\frac{1}{2}$ and

$$l=\tfrac{1}{2}\{-1+[1-4(\alpha+\beta)]^{1/2}\}. \quad (55)$$

Since the values of l for the physical case are restricted to $l\geqslant 0$ it is necessary that

$$\alpha+\beta\leqslant 0 \quad (56)$$

to have a limited range for l's.

Case A:

When $l(l+1)\leqslant-(\alpha+\beta)$.

In the class B^+B^-,

$$a_{l+}=1, a_{l-}=1. \quad (57)$$

In the class I^-B^+,

$$a_{l+}=1, a_{l-}=-(1/2\beta)[l(l+1)+\alpha]. \quad (58)$$

In the class I^+B^-,

$$a_{l-}=1, a_{l+}=-(1/2\beta)[l(l+1)+\alpha]. \quad (59)$$

In the class I^+I^-, if

$$-(\alpha+2\beta)\leqslant l(l+1)\leqslant-(\alpha+\beta),$$

$$a_{l+}=a_{l-}=-(1/2\beta)[l(l+1)+\alpha]. \quad (60)$$

If

$$l(l+1)<-(\alpha+2\beta) \quad (61)$$

the class I^+I^- is empty and does not contribute. This last case corresponds to

$$\alpha+2\beta\leqslant 0. \quad (62)$$

In case A the range of l is determined by the inequality (52).

Case B:

When $l(l+1)\geqslant-(\alpha+\beta)$.

In the class B^+B^-,

$$a_{l+}=0, a_{l-}=0 \quad (63)$$

In the class I^-B^+,

$$a_{l+}=0, a_{l-}=-(1/2\beta)[l(l+1)+\alpha]. \quad (64)$$

In the class I^+B^-,

$$a_{l-}=0, a_{l+}=-(1/2\beta)[l(l+1)+\alpha]. \quad (65)$$

In the class I^+I^- Eq. (23) is automatically satisfied and we have

$$a_{l+}=a_{l-}=-(1/2\beta)[l(l+1)+\alpha]. \quad (66)$$

In case B the range of l is determined from below by the inequality (53) and from above by vanishing of a_l's of the form (66). To minimize S one has to determine the parameters α and β from fitting of A_0 and E. For this, one has to choose amplitudes from different classes for the regions $l(l+1)<-(\alpha+\beta)$ and $l(l+1)>-(\alpha+\beta)$. Each choice gives a local minimum. For instance, if $A_0=E$, we have to choose the class B^+B^- for both regions since in this case the elasticity of all partial waves is known and the class B^+B^- represents elastic amplitudes. This gives $a_{l+}=a_{l-}=1$ for $l(l+1)<-(\alpha+\beta)$ and $a_{l+}=a_{l-}=0$ for $l(l+1)>-(\alpha+\beta)$. With these values one obtains for S

$$S=\tfrac{1}{2}A_0(A_0-1).$$

However, in general, this kind of information about the elasticity degree of the partial waves will not be available. If we choose for the first region the class B^+B^- and the second region I^+I^- we obtain

$$A=\sum_{B^+B}(2l+1)+\sum_{I^+I}(2l+1)[\alpha'-\beta'l(l+1)],$$

$$E=\sum_{B^+B}(2l+1)+\sum_{I^+I}(2l+1)[\alpha'-\beta'l(l+1)]^2.$$

Here we put $\alpha'=\alpha/2\beta$ and $\beta'=1/2\beta$.

It is seen that both the amplitudes and the constraints have exactly the same form as in the scalar case [case (a) of Ref. 3] and one obtains the result, Eq. (12), of MacDowell and Martin.

In the other combinations the elimination of the parameters in terms of A and E is complicated and the resulting formulas are not particularly illuminating. It may be better to do numerical calculations in specific cases. This will also be necessary to find the smallest and largest of minima.

IV. DISCUSSION

Using the variational technique with inequality constraints we looked at the problem of finding a lower bound for the forward slope in the spin 0–spin $\frac{1}{2}$ case when the total cross section, elastic cross section, and unitarity of the partial waves are used as constraints. We defined four classes such that a pair of amplitudes f_{l+}, f_{l-} for a given l belongs to one and only one of these classes depending on their elasticity or inelasticity.

The positivity of the Lagrange multipliers corresponding to the inequality constraints, together with the extremum conditions obtained from second variations are used to determine the forms of the partial waves in each class.

To minimize the forward slope the total cross section and the elastic cross section are fitted with the partial waves belonging to different classes. This fitting determines both the values of the l independent Lagrange multipliers and the range of l's. In general, numerical calculations may be necessary, but one of the solutions coincides with the result obtained previously for the scalar case.

The technique is quite general and we are planning to apply it to higher spin cases like the N–N problem. Obviously analytic solutions will be difficult to obtain. However numerical solutions may be of practical use.

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Proof of a Geroch conjecture[a)]

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We prove that any given stationary axisymmetric vacuum space-time (SAV) can be generated from Minkowski space by at least one Kinnersley–Chitre transformation, i.e., by at least one member of the Geroch group K, provided that the metric tensor and the Killing vectors are C^4 in a domain which covers at least one point of the axis at which one of the Killing vectors characterizing the space-time is timelike. We find that the set of all Kinnersley–Chitre transformations which map any given SAV into another given SAV is uniquely determined by the initial and final values of the Ernst potential on the axis. An explicit formula for these K-C transformations in terms of the initial and final axis values is given; this formula generalizes an analogous one which Xanthopoulos found for the asymptotically flat SAV's.

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1. INTRODUCTION

The central theme of this paper is the proof that any given stationary axially symmetric vacuum space-time can be generated from Minkowski space by a Kinnersley–Chitre[1-3] transformation, i.e., by a member of the Geroch[4,5] group K, provided that the space-time includes at least one point of the axis at which the matrix $h_{ab} := X_a \cdot X_b$ of scalar products of the Killing vectors X_3 and X_4 which characterize the space-time has rank 1 (as opposed to rank 0) and provided that X_a and g_{ab} are C^4 in a neighborhood of the point. The proofs of this theorem and of various related theorems demand that we first establish a substantial number of preliminary results concerning the complex plane representation of K introduced by the authors in two preceding papers,[6,7] which we shall designate as I and II. Some of these preliminary results are interesting in their own right; this is especially the case for a 2×2 matrix Fredholm equation of the second kind which will be derived in Sec. 4 and which provides a powerful analytical tool for investigating the properties of K-C (Kinnersley–Chitre) transformations.

To enable us to explain our objective more fully, it is advisable at this point to describe a few of the notations and conventions which we shall often use in this paper. The domain of our discourse is the set V of all stationary axially symmetric vacuum space-times. z and ρ will denote the Weyl canonical coordinates of any member of V, and R^2_+ will be the set of all (z,ρ) such that

$$-\infty < z < \infty, \quad 0 \leqslant \rho < \infty .$$

It is understood that the open subsets of R^2_+ are the intersections of R^2_+ with the open subsets of R^2, and continuity and derivatives of functions of (z,ρ) are defined in accordance with this topology. An Ernst potential of any given member of V will be expressed as a function $\mathcal{E}(z,\rho)$ of Weyl canonical coordinates *restricted to a domain* U such that U is a region (open connected set) in R^2_+, and such that

$$f := \operatorname{Re}\mathcal{E} > 0$$

at all points of U. We grant the manifold is C^∞ and that the metric tensor and Killing vectors are at least C^4; therefore, $\mathcal{E}$ is at least C^3. We shall let V_0 denote the set of all members of V for which $\mathcal{E}$-potentials exist, each of whose domains cover at least one point $(z_0, 0)$ of the axis; thus, $\mathcal{E}$ is at least C^3 in a neighborhood of $(z_0,0)$ and $f(z_0,0) > 0$. The asymptotically flat stationary axially symmetric vacuum space-times constitute a subset of V_0. After Sec. 3, whenever we have occasion to consider a member of V_0 in a neighborhood of a point $(z_0, 0)$ of the axis, it will be understood that the arbitrary constant in z is chosen so that $z_0 = 0$.

One of the important results in this paper is that $\mathcal{E}$ *is holomorphic in* U. To say that $\mathcal{E}$ is *holomorphic in* U means that $\mathcal{E}$ has an extension $[\mathcal{E}]$ to a region $[U]$ in $C \times C$ (where C is the complex plane) such that $[\mathcal{E}]$ is holomorphic in $[U]$; i.e., $[\mathcal{E}]$ is single-valued and is, in at least one neighborhood of each point of $[U]$, expressible as a Taylor series which converges to the function in that neighborhood. The holomorphy of $\mathcal{E}$ is proved in Sec. 2 and is based on the fact that if one of the two Killing vectors characterizing the space-time is timelike, (i.e., if $f > 0$ over U), then the real and imaginary parts of $\mathcal{E}$ constitute a solution of an *analytic elliptic system* of partial differential equations, and every C^3 solution of a system of this type is holomorphic.[8-10]

So far, we have said nothing about those vacuum space-times which are like the stationary axially symmetric ones except that both Killing vectors are spacelike; i.e., $f < 0$. To simplify our exposition, the bulk of this paper covers only the case where one of the Killing vectors is timelike. This involves no essential loss if generality since the corresponding equations and results for the other case are easily obtained by a few simple operations, which we shall provide in Sec. 6. The theorems and proof of the Geroch conjecture are also applicable in the case $f < 0$ *provided we assume that* $\mathcal{E}$ *is a holomorphic function of Weyl canonical coordinates.* (Holomorphy does not automatically follow when $f < 0$, since the equation governing $\mathcal{E}$ is then hyperbolic.) This assumption is viable since Theorem 4, which we shall prove in Sec. 5, guarantees as one of its conclusions that *the holomorphy of* $\mathcal{E}$ (but not necessarily the domain) *is preserved by* K-C *transformations.*

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That completes our preliminary account of notations and conventions. The term stationary axially symmetric space-time will be abbreviated SAV.

The motivation behind our principal objective has its origins in work of Geroch and of Kinnersley and Chitre. One of the intriguing ideas in general relativity over the past decade has been the conjecture advanced by Geroch[4,5] that a substantial subset of V (including all of its asymptotically flat members) can be obtained from Minkowski space by an infinite-dimensional Lie group K of transformations, whose underlying symmetry is the free product of the group of $SL(2,R)$ transformations of the pair of Killing vectors characterizing V and of an internal $SU(1,1)$ symmetry of the second order differential equation which defines $\mathcal{E}$. This idea remained academic until K-C created a workable representation of the Lie algebra of K plus various techniques which could actually be used to compute hitherto unknown *interesting* members of V from those which are already known.[1-3]

Since then, results of Hoenselaers, Kinnersley, and Xanthopoulos[11] and Xanthopoulos[12] have lent further credence to the Geroch conjecture insofar as the asymptotically flat members of V are concerned. Their work strongly suggests that any given asymptotically flat member S of V_0 can be generated from MS (Minkowski space) by applying two successive transformations belonging respectively to two specific abelian subgroups K_0 and K_1 of K. These subgroups shall be defined in Sec. 4. The first transformation $u^{(0)}$ maps MS into an asymptotically flat Weyl space-time S^W, and the second transformation $u^{(1)}$ maps S^W into S.

An especially noteworthy recent development has been the discovery by Xanthopoulos[12] that the axis values $\mathcal{E}(z,0)$ of the $\mathcal{E}$-potential of S uniquely determine (for a specific choice of gauge) the transformations $u^{(0)}$ and $u^{(1)}$ in accordance with simple algebraic relations which he derived. As Xanthopoulos noted, and as we shall make clear in Sec. 5, this brings us closer than ever before to a proof of the Geroch conjecture for the asymptotically flat SAV's. One of the key results in our paper is an extension of the Xanthopoulos result to V_0 and to arbitrary members of K which map V_0 into V_0. Specifically, if $u(t)$ denotes our 2×2 matrix representation of *any element* of K which induces the transformation

$$\mathcal{E}^{(0)}(z,\rho)\rightarrow \mathcal{E}(z,\rho)$$

of the $\mathcal{E}$-potential, then we shall prove that[13]

$$\mathcal{E}(z,0)\mathcal{E}^{(0)}(z,0)ku_3^4(k)+k^{-1}u_4^3(k)$$
$$+i\mathcal{E}(z,0)u_4^4(k)-i\mathcal{E}^{(0)}(z,0)u_3^3(k)=0\,, \qquad (1)$$

$k:=(2z)^{-1}$, u_b^a: = entry in ath row and bth column of u.

The above result enables us to find the family of all K-C transformations (in our representation) which map any given member of V_0 into any given member of V_0. We shall derive Eq. (1) in Sec. 5, and we shall use Eq. (1) in Sec. 5 to help us establish *our principal result which is, in a certain sense, a proof of the Geroch conjecture*. More specifically, we shall prove the following theorem:

Theorem 1: *Any member of V_0 can be obtained from* MS *by at least one transformation in a subgroup* $\mathcal{K}$ *of* K.

Conversely, any element of $\mathcal{K}$ *transforms* MS *into a member of* V_0.

Our representation of $\mathcal{K}$ will be defined in Sec. 4.

As we pointed out in our opening sentences, the task of proving our version of the Geroch conjecture involves a large number of preliminary concepts and theorems. We shall proceed according to a definite plan, which we now outline.

In Sec. 2, we shall prove a few pertinent results concerning that generalization of the $\mathcal{E}$-potential which we call the *H-potential*, which was originally introduced[1,2] by K-C, and which was defined and extensively discussed[7] in II. The key result of Sec. 2 will be an explicit general solution for *H on the axis* for any SAV in V_0.

In Sec. 3, we shall prove a few pertinent results concerning that generalization of the H-potential which we call the *F-potential*, which was originally introduced[2] by K-C as a generating function for part of their hierarchy of potentials, and which was defined and extensively discussed[7] in II. *It is precisely the F-potentials which constitute the domain of our representation of the Geroch group.* Each F-potential is a 2×2 matrix function $F(z,\rho,t)$ of a complex variable t as well as of z and ρ. The key results in Sec. 3 will be as follows.

(a) An explicit general solution for $F(z,0,t)$ for any SAV in V_0.

(b) A theorem which asserts that the gauge of the F-potentials for members of V_0 can be chosen so that the only singularities of $F(z,\rho,t)$ in the complex t-plane are at

$$t=[2(z\pm i\rho)]^{-1}\,,$$

and such that, when $z^2+\rho^2\neq 0$,

$$F(z,\rho,t)\begin{pmatrix} t & 0\\ 0 & 1\end{pmatrix}$$

is holomorphic and has an inverse at $t=\infty$. Moreover, specifics concerning the holomorphy of $F(z,\rho,t)$ with respect to all three variables will be given. These specifics are required for the proofs of some crucial theorems in Secs. 4 and 5.

In Sec. 4, we shall explain our representation of K and give three equivalent methods of effecting K-C transformations. The first of these methods is a homogeneous Hilbert problem,[7] which was introduced and discussed in II; we shall use this homogeneous Hilbert problem to help fix our gauge. The second method is a linear integral equation of the Cauchy type,[6] which was introduced and discussed in I; we shall give an alternative form of this equation which suits our present purpose and which will be used, in Sec. 5, to derive Eq. (1). The third method of effecting K-C transformations is the Fredholm equation of the second kind which was mentioned in our opening sentences and which will be used to prove one of the theorems in Sec. 5.

This theorem will establish the correctness of one of the two hypotheses[7] which were assumed (without proof) in II and which are basic existence conditions for the K-C transformations. For transformations of V_0 into V_0, the other hypothesis and Eq. (1) will then be proved and will be used, in turn, to prove our version (Theorem 1) of the Geroch conjecture.

In Sec. 6, we shall discuss some of the problems which remain to be tackled and which are linked to the Geroch conjecture.

2. THE *H*-POTENTIAL

The *H-potential* is a 2×2 matrix field

$$H=\begin{pmatrix} H_{33} & H_{34} \\ H_{43} & H_{44}\end{pmatrix}$$

which may be defined as that solution of the equations

$$-i\rho H_z = h\epsilon H_\rho, \quad i\rho H_\rho = h\epsilon H_z,$$
$$H_z := \partial H/\partial z\,, \quad H_\rho := \partial H/\partial\rho\,, \tag{2}$$

such that

$$h=-\mathrm{Re}\,H\,, \quad \epsilon := \begin{pmatrix} 0 & 1 \\ -1 & 0\end{pmatrix}, \tag{3}$$

where h is the 2×2 symmetric real matrix whose elements h_{ab} are the metric components in the line element

$$e^{2\Gamma}(\delta z^2+\delta\rho^2)+h_{ab}\delta x^a\delta x^b$$
$$(a,b=3,4) \tag{4}$$

of the given SAV. Above Γ and h depend at most on z and ρ, which are defined by the equations

$$\rho^2=-\det h\,, \quad 2iz\epsilon = H-H^T\,. \tag{5}$$

The H-potential is not uniquely defined by Eqs. (2) and (3). It remains arbitrary up to the transformation

$$H\to H+iB\,, \tag{6}$$

where B is any real 2×2 constant matrix. Also, if the ignorable coordinates x^a are subject the GL$(2,R)$ transformation

$$\begin{pmatrix} x^3 \\ x^4\end{pmatrix} \to S^{-1}\begin{pmatrix} x^3 \\ x^4\end{pmatrix}, \quad dS=0\,,$$

then

$$H\to S^T HS\,. \tag{7}$$

From Eqs. (3) and (5), Eqs. (6) and (7) imply the corresponding transformations

$$z\to z+\tfrac{1}{2}(B_{34}-B_{43})\,,$$
$$\rho\to(\det S)\rho\,, \quad z\to(\det S)z\,. \tag{8}$$

For any given SAV, we generally use the transformation (7) to make $h_{44}<0$ at some given point, and we restrict H to a region which contains the point and in which h_{44} has no zeros. We then define

$$\mathcal{E} := H_{44}\,, \quad f := \mathrm{Re}\,\mathcal{E} = -h_{44}\,, \tag{9}$$

whereupon it is clear that $f>0$ throughout the domain of H. With the aid of Eqs. (3) and (5), the well-known basic field equation[14] which governs the $\mathcal{E}$-potential may be deduced from the integrability condition for Eq. (2); it is

$$\mathcal{E}_{\rho\rho}+\rho^{-1}\mathcal{E}_\rho+\mathcal{E}_{zz}=f^{-1}(\mathcal{E}_\rho^2+\mathcal{E}_z^2)\,. \tag{10}$$

The metric field Γ in Eq. (4) is determined by the equations

$$\gamma_z=\tfrac{1}{4}\rho f^{-2}(\mathcal{E}_z\mathcal{E}_\rho^*+\mathcal{E}_\rho\mathcal{E}_z^*)\,,$$
$$\gamma_\rho=\tfrac{1}{4}\rho f^{-2}(-\mathcal{E}_z\mathcal{E}_z^*+\mathcal{E}_\rho\mathcal{E}_\rho^*)\,, \tag{11}$$

where

$$\exp(2\gamma) := f\exp(2\Gamma)\,.$$

Also, as is well known, *all elements of* H *including the metric tensor are uniquely determined by* $\mathcal{E}$ *up to a gauge transformation.* The pertinent equations, which are derived from Eqs. (2), (3), and (5), are

$$J := \mathrm{Im}\,H\,, \quad \chi := J_{44}=\mathrm{Im}\,\mathcal{E}\,,$$
$$(f^{-1}h_{34})_\rho = -\rho f^{-2}\chi_z\,, \quad (f^{-1}h_{34})_z=\rho f^{-2}\chi_\rho\,,$$
$$(J_{34})_\rho = -f^{-1}(\rho f_z + h_{34}\chi_\rho)\,,$$
$$(J_{34})_z = f^{-1}(\rho f_\rho - h_{34}\chi_z)\,, \tag{12}$$
$$(J_{33})_\rho = f^{-1}[2\rho(h_{34})_z - h_{33}\chi_\rho]\,,$$
$$(J_{33})_z = f^{-1}[2h_{34}-2\rho(h_{34})_\rho - h_{33}\chi_z]\,,$$
$$h_{33}=f^{-1}[\rho^2-(h_{34})^2]\,, \quad J_{43}=J_{34}-2z\,.$$

Clearly, Eqs. (3), (11), and (12) uniquely define a SAV for any given solution $\mathcal{E}$ of Eq. (10). *It is also clear that* γ, h, *and* H *are holomorphic if* $\mathcal{E}$ *is holomorphic.* ($\mathcal{E}$ is holomorphic if and only if both f and χ are holomorphic.)

For any given SAV, *it is automatically true that* $\mathcal{E}$ *is holomorphic.* To prove this, we shall first show that f and χ are real analytic functions in at least one neighborhood of any given point (z_0,ρ_0) of U such that $\rho_0>0$. Let ψ be the real-valued function

$$\psi := \tfrac{1}{2}\ln f\,.$$

Then, Eq. (10) is equivalent to the pair of equations

$$\psi_{\rho\rho}+\rho^{-1}\psi_\rho+\psi_{zz}+\tfrac{1}{2}[\exp(-4\psi)](\chi_\rho^2+\chi_z^2)=0\,,$$
$$\chi_{\rho\rho}+\rho^{-1}\chi_\rho+\chi_{zz}-4(\psi_\rho\chi_\rho+\psi_z\chi_z)=0\,,$$

which constitute an elliptic system of partial differential equations with left-hand sides which are analytic functions of $(z,\rho,\psi,\psi_\rho,\psi_z,\chi_\rho,\chi_z,\psi_{\rho\rho},\psi_{zz},\chi_{\rho\rho},\chi_{zz})$ over the domain $N\times R^9$, where $N\subset U$ is any connected neighborhood of (z_0,ρ_0) such that $\rho>0$ whenever $(z,\rho)\in N$. Therefore, from a general theorem[8-10] concerning such *analytic elliptic systems*, if ψ and χ are C^3 solutions, then ψ and χ are real analytic in N. It follows that f and χ are real analytic at all off-axis points of U.

The above argument does not work for a point $(z_0,0)\in U$. We shall handle this case by introducing three independent variables

$$x=\rho\cos\phi\,, \quad y=\rho\sin\phi,\ z\,,$$

where $0\leqslant\phi<2\pi$. Let T_U denote the set of all

$$(\rho\cos\phi,\ \rho\sin\phi,\ z)$$

in R^3 such that $0 \leq \phi < 2\pi$ and $(z,\rho)\in U$. Let σ and α denote those functions which each have the domain T_U and which have values given by

$$\sigma(x,y,z) := \psi(z,(x^2+y^2)^{1/2}),$$

$$\alpha(x,y,z) := \chi(z,(x^2+y^2)^{1/2}).$$

Suppose ψ and χ are C^3 functions at all points of U including points on the axis. From Eq. (10), we obtain

$$\psi_\rho(z,0)=\chi_\rho(z,0)=\psi_{\rho\rho\rho}(z,0)=\chi_{\rho\rho\rho}(z,0)=0$$

for all $(z,0)$ in U. With the aid of the above values, we can then prove that σ and α are C^3 functions at all points of T_U including points $(0,0,z)$ on the axis; moreover, Eq. (10) is equivalent to the pair of equations

$$\nabla^2\sigma + \tfrac{1}{2}[\exp(4\sigma)](\nabla\alpha)^2 = 0,$$

$$\nabla^2\alpha - 4(\nabla\sigma)\cdot(\nabla\alpha) = 0,$$

subject to the conditions of axial symmetry

$$(\partial/\partial\phi)\sigma = (\partial/\partial\phi)\alpha = 0.$$

Above, ∇ and ∇^2 are the three-dimensional Euclidean space gradient and Laplacian operators. The pair of second-order equations in σ and α is obviously an *analytic elliptic system*. Hence, σ and α are real analytic at all points of T_U; in particular, there exist Taylor series expansions of σ and α about the point $(0,0,z_0)$ such that these series converge to the functions in at least one neighborhood of $(0,0,z_0)$. The subsidiary conditions of axial symmetry then clearly imply that there exists a neighborhood $N \subset U$ of the point $(z_0,0)$ such that ψ and χ have series expansions

$$\psi = \sum a_{mn}(z-z_0)^m\rho^{2n}, \quad \chi = \sum b_{mn}(z-z_0)^m\rho^{2n},$$

which converge to the respective functions at all (z,ρ) in N. The above series can be extended to negative values of ρ by means of the formal device

$$\psi(z,-\rho) := \psi(z,\rho), \quad \chi(z,-\rho) := \chi(z,\rho).$$

In summary, we have proved that any C^3 solution of Eq. (10) is an analytic function of real (z,ρ) at all points of U. Therefore,[15] it is also holomorphic in the sense defined in Sec. 1. *That completes our proof.*

Our primary interest in this paper is the set of SAV's which are members of V_0. *For them, H is holomorphic in a neighborhood of a point $(z_0,0)$ on the axis.* As is easily shown, we can use the transformations (6) and (7) to make

$$H(z_0,0) = \begin{pmatrix} 0 & 0 \\ -2iz_0 & \mathcal{E}(z_0,0) \end{pmatrix}. \tag{13}$$

Then, by a straightforward process, we may use Eqs. (10) and (12) to deduce the following results for $H(z,0)$ and $H_\rho(z,0)$ in that maximum interval of the z axis which contains z_0 and on which $f(z,0)>0$:

$$H(z,0) = \begin{pmatrix} 0 & 0 \\ -2iz & \mathcal{E}(z,0) \end{pmatrix}, \tag{14}$$

$$H_\rho(z,0) = 0. \tag{15}$$

Equations (14) and (15) will play a key role in the next section.

3. THE F-POTENTIALS

A. Defining equations and gauge transformations

The domain which is transformed by our representation of K is a set of 2×2 matrix functions F of z, ρ, and a complex variable t. These *F-potentials* were originally introduced by K-C as generating functions for part of their hierarchy of potentials.[2] The F-potentials, their gauge, and their singularities were discussed in some detail in II.[7]

Corresponding to any given H-potential whose domain is U, the domain[16] of F is a region Δ in the space $U\times C$, where the complex plane C is understood to include $t=\infty$ (and, therefore, to have the topology of the Riemann sphere). We let[16]

$$\mathbf{x} := (z,\rho),$$

and, for each t in C, we define

$$\Delta_t := \text{set of all } \mathbf{x} \text{ in } U \text{ such that } (\mathbf{x},t) \text{ is in } \Delta.$$

Δ is not arbitrary; e.g., the domain must be chosen so that F is single-valued. At the same time, Δ is not unique. We shall have more to say about suitable choices for Δ later in this section. In the meantime, we grant that Δ is given, and *we let $F(t)$ denote that function whose domain is Δ_t and whose value at each point $\mathbf{x}$ in Δ_t is $F(\mathbf{x},t)$.*

For given H, we define F as any solution of the differential equation

$$dF = \Gamma\Omega F \quad (\Omega := i\epsilon) \tag{16}$$

subject to the subsidiary conditions that F be (for fixed $\mathbf{x}$) holomorphic in a neighborhood of $t=0$ and that $F(t)$ satisfy

$$F(0)=\Omega, \quad \dot{F}(0)=H,$$

$$\det F(t) = -\lambda(t)^{-1}, \tag{17}$$

$$F(t)^\dagger[\Omega - t\Omega(H+H^\dagger)\Omega]F(t) = \Omega.$$

Above, Γ is the 1-form

$$\Gamma = -\frac{1}{2}\left(\frac{dr_+}{r_+-\tau}\frac{\partial H}{\partial r_+} + \frac{dr_-}{r_--\tau}\frac{\partial H}{\partial r_-}\right), \tag{18}$$

where

$$r_\pm := z \pm i\rho, \quad \tau := (2t)^{-1}$$

$$\partial/\partial r_\pm = \tfrac{1}{2}(\partial/\partial z \mp i\partial/\partial\rho). \tag{19}$$

Also,

$$\dot{F}(t) := \partial F(t)/\partial t,$$

$$F(t)^\dagger := \text{h.c. (Hermitian conjugate) of } F(t^*),$$

and

$$\lambda(t) := [(1-2tz)^2 + (2t\rho)^2]^{1/2}. \tag{20}$$

Equations (2) and (5) imply that Eq. (16) is completely integrable.[7] As regards the subsidiary conditions of Eqs. (17), we proved in II that these conditions are consistent with Eq. (16).[7]

Equations (16) and (17) do not define F uniquely. If F is any given solution, so is[7]

$$F' = Fv, \tag{21}$$

where v is any 2×2 matrix function of t (independent of $\mathbf{x}$) such that v is holomorphic in a neighborhood of $t=0$, and

$$v(0)=I, \quad \dot{v}(0)=0,$$
$$v(t)^\dagger \epsilon v(t)=\epsilon, \quad \det v(t)=1. \tag{22}$$

For given H, Eq. (21) is the general gauge transformation of the F-potential. Each gauge transformation may be accompanied by a change in the domain of the F-potential; i.e., the domain Δ' of F' may differ from the domain Δ of F.

It is desirable to restrict the gauge to one for which the set of *t-plane singularities* of the F-potential is minimized. Let U_Δ denote the set of all points $\mathbf{x}$ in U such that $(\mathbf{x}, t)$ is a member of Δ for at least one point t in C. For given $\mathbf{x}$ in U_Δ, let

$$t(\mathbf{x}) := (2r_-)^{-1}, \quad t(\mathbf{x})^* := (2r_+)^{-1}. \tag{23}$$

In II, we proved that, for fixed $\mathbf{x}$ in U_Δ, the F-potential has t plane singularities at $t(\mathbf{x})$ and $t(\mathbf{x})^*$ regardless of the choice of gauge.[7] These are branch points of index $-\frac{1}{2}$ when $\rho>0$; when $\rho\to 0$, the points merge to form a simple pole. Also, we proved that the gauge can be chosen so that, if $z^2+\rho^2\neq 0$,

$$F(t)\begin{pmatrix} t & 0\\ 0 & 1\end{pmatrix} \tag{24}$$

is holomorphic at $t=\infty$, and such that the only other singularities (if they occur at all) are at two conjugate fixed branch points $t(\mathbf{x}_0)$ and $t(\mathbf{x}_0)^*$ of index $-\frac{1}{2}$. In this gauge, the set

$$\Delta_\mathbf{x} := \{t\in C : (\mathbf{x}, t)\in \Delta\}$$

is C minus $\{t(\mathbf{x}), t(\mathbf{x})^*\}$, possibly minus $\{t(\mathbf{x}_0), t(\mathbf{x}_0)^*\}$, and minus 0, 1, or 2 branch cuts which do not pass through $t=0$ or $t=\infty$. For fixed $\mathbf{x}$, F is a holomorphic function of t at all points of $\Delta_\mathbf{x}$. For fixed t, F is a holomorphic function of $\mathbf{x}$ at all points of

$$\Delta_t := \{\mathbf{x}\in U_\Delta : (\mathbf{x}, t)\in \Delta\}.$$

We shall now examine the entire question of the gauge for SAV's in V_0. It is our intention, for this case, to establish a stronger result than the one in II; viz., *we are going to show that the gauge can be selected so that the only singularities are those given by* Eq. (23). *In this gauge,* $\Delta_\mathbf{x}$ *is C minus the points* $t(\mathbf{x})$ *and* $t(\mathbf{x})^*$ *and minus a cut (line)* $K_\mathbf{x}$ *which joins* $t(\mathbf{x})$ *to* $t(\mathbf{x})^*$.

The first step is to remove the vagueness concerning the domain of the F-potential of any given SAV in V_0. This does not mean that we are going to lay down rules for constructing all possible F-potential domains of the given SAV. However, we shall introduce a class of *admissible F-potential domains* which can be used in practice and which will serve all present purposes. (In Sec. 5, we shall consider other F-potential domains.)

B. Some F-potential domains

We start with a simple example of an admissible domain. Then we shall generalize this example in two successive stages.

Consider any SAV in V_0, and recall that there exists at least one point $(z_0, 0)$ of the axis which is contained in the domain U of the H-potential. Select the arbitrary constant in z so that $z_0=0$. Then there exists at least one r_Δ = a positive real number or ∞ such that the set U_Δ of all (z,ρ) for which

$$z=r\cos\theta, \quad \rho=r\sin\theta,$$
$$0\leq r<r_\Delta, \quad 0\leq\theta\leq\pi, \tag{25}$$

is a subset of U. For any point $\mathbf{x}$ in U_Δ corresponding to given (r,θ), let

$$\mathbf{l}(\mathbf{x}) := \{(r\cos\theta', r\sin\theta') : \theta\leq\theta'\leq\pi\}, \tag{26}$$
$$K_\mathbf{x} := \{t\in C : \mathbf{x}_t\in \mathbf{l}(\mathbf{x})\}, \tag{27}$$
$$\Delta_\mathbf{x} := C - K_\mathbf{x}, \tag{28}$$

where $\mathbf{x}_t$ denotes that point in R_+^2 which is defined by

$$\mathbf{x}_t := (z_t, \rho_t) := (\mathrm{Re}\,\tau, |\mathrm{Im}\,\tau|). \tag{29}$$

Note that $\mathbf{l}(\mathbf{x})$ is an arc in U_Δ which joins $(-r,0)$ to $\mathbf{x}$, whereas $K_\mathbf{x}$ is an arc in C which joins $t(\mathbf{x})$ to $t(\mathbf{x})^*$. In the special case when $z<0$ and $\rho=0$, $K_\mathbf{x}$ is a singlet; when $z>0$ and $\rho=0$, $K_\mathbf{x}$ is a singlet; when $z>0$ and $\rho=0$, $K_\mathbf{x}$ is a closed contour about the origin; when $z=\rho=0$, $K_\mathbf{x}=\{\infty\}$. One *admissible F-potential domain* Δ is given by

$$\Delta = \{(\mathbf{x}, t) : \mathbf{x}\in U_\Delta, t\in\Delta_\mathbf{x}\}. \tag{30}$$

To gain some further perception of Δ, consider any given point t in C, and let

$$K_t := \{\mathbf{x}\in U_\Delta : r=r_t, 0\leq\theta\leq\theta_t\}, \tag{31}$$
$$\Delta_t := U_\Delta - K_t, \tag{32}$$

where r_t and θ_t are defined by

$$z_t = r_t\cos\theta_t, \quad \rho_t = r_t\sin\theta_t.$$

If $\mathbf{x}_t$ is not in U_Δ, then K_t is empty by definition. Otherwise, K_t is an arc in U_Δ which joins $\mathbf{x}_t$ to a boundary point of U_Δ; this arc degenerates to a point when $\theta_t=0$ or $r_t=0$ (real positive t or $t=\infty$). Note that Δ_t is a simply connected subregion of U_Δ except when t is real and negative within bounds such that $-r_\Delta<z_t<0$; in the exceptional case,[17] Δ_t consists of two disjoint simply connected components separated by K_t. It is easily seen that Δ is a simply connected subregion of $U\times C$.

We next slightly generalize the above choice of Δ. Suppose that the set of (z,ρ) given by Eqs. (25) is contained in U with the possible exception of a closed subset of the positive z axis. (Of course, the use of the term positive as opposed to negative is arbitrary; the roles of the positive and negative z axes may be interchanged if obvious suitable alterations are made in our definitions of $\mathbf{l}(\mathbf{x})$, $K_\mathbf{x}$, and K_t.) Then, we simply define U_Δ as the set of all $\mathbf{x}$ which are given by Eqs. (25) *and which are also members of U*. The definitions (26) to (32) and the remarks which accompany these definitions remain in force; the only changes are those induced by the fact that $(z,0)$ need no longer be a member of U_Δ when $z > 0$.

In the special case of a member of V_0 for which the arbitrary constant in z can be chosen so that U includes all of R^2_+ except perhaps for points on the positive z axis, we may choose $r_\Delta = \infty$ in Eqs. (25), whereupon $U_\Delta = U$. Except for this special case, U_Δ as defined above has a semicircular boundary in R^2_+. This severe restriction on the shape of U_Δ will now be dropped by replacing Eqs. (25) with the more general forms

$$z = Z(\xi,\eta), \quad \rho = P(\xi,\eta), \tag{33}$$

where Z and P are any C^∞ (i.e., have C^∞ extensions to regions in R^2) functions of real parameters ξ, η over the domain

$$0 < \xi < r_\Delta, \quad 0 \le \eta \le 1, \tag{34}$$

such that

$$\begin{aligned} &Z(\xi,0) = -\xi, && P(\xi,0)=0 \quad \text{for all } \xi, \\ &Z(\xi,1) > 0, && P(\xi,1)=0 \quad \text{for } \xi > 0, \\ &Z(0,\eta) = P(0,\eta) = 0 && \qquad\qquad \text{for all } \eta, \end{aligned} \tag{35}$$

such that

$$\frac{1}{\xi}\left(\frac{\partial Z}{\partial \xi}\frac{\partial P}{\partial \eta} - \frac{\partial Z}{\partial \eta}\frac{\partial P}{\partial \xi}\right) \neq 0 \text{ and is } C^\infty \text{ for all } \xi, \eta, \tag{36}$$

such that the values of (z,ρ) given by Eqs. (33) and (34) are members of U whenever $\eta < 1$, and such that those values which correspond to $\eta = 1$ constitute a half-open interval of the axis which has $(0,0)$ as a left-hand end point. As an example, Eqs. (25) are expressible in the form

$$z = -\xi\cos\pi\eta, \quad \rho = \xi\sin\pi\eta.$$

We now let U_Δ denote the set of all values of (z,ρ) given by Eqs. (33) and (34) such that (z,ρ) is a member of U. Note that U_Δ is a simply-connected region in R^2_+ and that its boundary contains an open interval of the axis consisting of all $(z,0)$ such that

$$-r_\Delta < z < \bar{r}_\Delta, \quad (z,0) \in U_\Delta, \tag{37}$$

where $\bar{r}_\Delta > 0$ (and may be ∞) and $(\bar{r}_\Delta, 0)$ is not itself a member of U_Δ. Of course, there may be other open intervals of the axis which are contained in U_Δ but which have $z > \bar{r}_\Delta$. For any point $\mathbf{x}$ in U_Δ corresponding to given (ξ,η), we let

$$\mathbf{1}(\mathbf{x}) := \{(Z(\xi,\eta'), P(\xi,\eta')) : 0 \le \eta' \le \eta\}, \tag{38}$$

which is clearly an arc in U_Δ which joins the point $(-\xi, 0)$ to the point $\mathbf{x}$. The definitions (27), (28), and (30) of $K_\mathbf{x}$, $\Delta_\mathbf{x}$, and Δ remain in force, as do the remarks between Eqs. (29) and (30). For any given point t in C, we let

$$K_t := \{\mathbf{x} \in U_\Delta : z = Z(\xi_t, \eta), \quad \rho = P(\xi_t,\eta), \quad \eta_t \le \eta \le 1\}, \tag{39}$$

where (ξ_t, η_t) is a value of (ξ,η) such that

$$z_t = Z(\xi_t,\eta_t), \quad \rho_t = P(\xi_t, \eta_t).$$

$\mathbf{x}_t = (z_t, \rho_t)$ and Δ_t are defined as before by Eqs. (29) and (32), and the statements which follow these equations also remain in force (except that $\theta_t = 0$ is replaced by $\eta_t = 1$, and $r_t = 0$ is replaced by $\xi_t = 0$); in particular, Δ is a simply connected subregion of $U \times C$.

$\mathfrak{D}_0$ will denote the set of all F-potential domains as defined above. If $\mathbf{x}$ is any given point in U, then it is clear that there exists at least one choice of the origin $(0,0)$ and of the functions Z and P in Eqs. (33) such that thecorresponding U_Δ covers $\mathbf{x}$. This feature makes $\mathfrak{D}_0$ adequate for all applications.

C. The F-potential on the axis

The next step is to pin down F uniquely for given H and given $\Delta \in \mathfrak{D}_0$. To do this, we shall take advantage of the fact that the explicit form of the general solution for F along the axis ($\rho = 0$) can be obtained; we shall pin down F uniquely by selecting a specific solution for $F(z,0,t)$ over a domain [see Eqs. (19) and (29)]

$$\begin{aligned} \mathcal{I} := &\{(z,t) : t \in C, \ -r_\Delta < z < 0\} \\ &- \{(z_t, t) : t = \infty \text{ or } t = \text{real}, \ -r_\Delta < z_t < 0\}. \end{aligned} \tag{40}$$

From Eqs. (18) to (20), we may show that Eq. (16) is equivalent to the pair of partial differential equations

$$\begin{aligned} F_z(t) &= t\lambda(t)^{-2}[(1-2tz)H_z + 2t\rho H_\rho]\,\Omega F(t), \\ F_\rho(t) &= t\lambda(t)^{-2}[(1-2tz)H_\rho - 2t\rho H_z]\,\Omega F(t). \end{aligned} \tag{41}$$

With the aid of Eqs. (14) and (15), the second of the above equations implies

$$F_\rho(z,0,t) = 0 \text{ for all } (z,0,t) \text{ in } \Delta, \tag{42}$$

and the first of Eqs. (41) can be integrated along the axis. The reader can easily verify that one solution for $F(z,0,t)$ which has the domain $\mathcal{I}$, which is (for fixed z) holomorphic in a neighborhood of $t=0$, and which satisfies all of the Eqs. (17) is given by

$$F(z,0,t) = \begin{pmatrix} 0 & i \\ \dfrac{-i}{1-2tz} & \dfrac{t\,\mathcal{E}(z,0)}{1-2tz} \end{pmatrix}. \tag{43}$$

The above expression is also valid for at least some (z,t) such that $z > 0$, but we do not have to know its maximal domain and need not further concern ourselves with extensions of Eqs. (43) to positive z until Theorem 5 in Sec. 5. To gain some perception of the domain $\mathcal{I}$, consider any given point t in C, and let

$$\mathcal{I}_t := \{z : (z,t) \in \mathcal{I}\}. \tag{44}$$

If t is not real or if t is real such that $t > 0$ or $2tr_\Delta < -1$, then $\mathcal{I}_t$ is the connected interval $-r_\Delta < z < 0$. If $t = \infty$, then $\mathcal{I}_t$ is the connected interval $-r_\Delta < z < 0$. However, if t is real and $-r_\Delta < z_t < 0$, then $\mathcal{I}_t$ consists of two disjoint connected intervals separated by the point z_t; the connection between the values of F on the two sides of z_t is provided by analytic continuation of the F-potential expressed as a function of t in $\Delta_\mathbf{x}$ for any given $\mathbf{x} = (z,0)$ such that $-r_\Delta < z < 0$.

D. Holomorphy of F

We are now ready to state the key result of this section.

Theorem 2: *Consider any given H-potential H for a member of* V_0 *and any given* Δ *in* $\mathfrak{D}_0$. *There exists exactly one solution F of Eqs.* (16) *and* (17) *such that the domain of F is* Δ *and such that the values of F over the set* $\mathcal{G}$ [Eq. (40)] *are given by Eq.* (43). *This solution is a holomorphic function of* (z, ρ, t) *at all points of* Δ, *and, for fixed* $(z,\rho) \neq (0,0)$,

$$F(t)\begin{pmatrix} t & 0 \\ 0 & 1 \end{pmatrix} \tag{45}$$

is holomorphic at $t=\infty$ *and has an inverse there. Furthermore, for given* $\mathbf{x}=(z,\rho)$ *in* U_Δ *such that* $\rho>0$, $t(\mathbf{x})$ *and* $t(\mathbf{x})^*$ *are branch points of index* $-\frac{1}{2}$, *and the section* $\Delta_\mathbf{x}$ *of the domain is the complex plane minus these branch points and minus the cut* $K_\mathbf{x}$ *which joins them.*[18]

The objects $t(\mathbf{x})$, $K_\mathbf{x}$, and $\Delta_\mathbf{x}$ in the above theorem were defined by Eqs. (23), (27), (28), and (38). The last sentence in the theorem is a repetition of material covered in II and of the definition of $\Delta_\mathbf{x}$. We shall now sketch the proof of those parts of the theorem which precede the last sentence, but we shall omit various details which can be obtained from II.[7] The proof will be given in five steps.

(1) First, we consider any given value of t such that *it is not true* that t is real and $-r_\Delta < z_t < 0$. Then, Δ_t is simply connected. [See Eqs. (29) to (32).]

Let $\mathfrak{F}(t)$ denote that function[19] whose domain is $\Delta_t \times \Delta_t$ and which satisfies, for all $\mathbf{x}$ and $\mathbf{y}$ in Δ_t,

$$d\mathfrak{F}(\mathbf{x},\mathbf{y},t)=\Gamma(\mathbf{x},t)\,\Omega\mathfrak{F}(\mathbf{x},\mathbf{y},t),$$

$$\mathfrak{F}(\mathbf{y},\mathbf{y},t)=I, \tag{46}$$

where $\Gamma(\mathbf{x},t)$ is defined by Eq. (18). From theorems proved[7] in an Appendix of II, $\mathfrak{F}(t)$ exists, is unique, is holomorphic over its domain $\Delta_t\times\Delta_t$ (meaning that it has a holomorphic extension to a region in C^4), and

$$\mathfrak{F}(\mathbf{x},\mathbf{y},t)\mathfrak{F}(\mathbf{y},\mathbf{w},t)=\mathfrak{F}(\mathbf{x},\mathbf{w},t) \tag{47}$$

for all $\mathbf{x}, \mathbf{y}, \mathbf{w}$ in Δ_t.

Also, with the aid of Eqs. (46), we prove that

$$\mathfrak{F}(\mathbf{x},\mathbf{y},0)=I,\quad \dot{\mathfrak{F}}(\mathbf{x},\mathbf{y},0)=[H(\mathbf{x})-H(\mathbf{y})]\,\Omega,$$

$$\det\mathfrak{F}(\mathbf{x},\mathbf{y},t)=\lambda(\mathbf{x},t)^{-1}\lambda(\mathbf{y},t),$$

$$\mathfrak{F}(\mathbf{x},\mathbf{y},t)^\dagger\{\Omega-t\Omega[H(\mathbf{x})+H(\mathbf{x})^\dagger]\,\Omega\}\,\mathfrak{F}(\mathbf{x},\mathbf{y},t)$$

$$=\Omega-t\Omega[H(\mathbf{y})+H(\mathbf{y})^\dagger]\,\Omega, \tag{48}$$

where $\lambda(\mathbf{x},t)$ is defined by Eq. (20). [To prove the above relations, note that Eqs. (59) to (61) of II remain valid if $\mathfrak{F}(\mathbf{x},\mathbf{y},t)$ replaces $F(\mathbf{x},t)$ and $H\Omega$ replaces H in these equations.[7] From Eqs. (59)–(61) of II and from the second of Eqs. (46), we can readily obtain Eqs. (48).]

Next, let

$$G(\mathbf{x},t):=\mathfrak{F}(\mathbf{x},\mathbf{x}_1,t)F(\mathbf{x}_1,t),$$

$$\mathbf{x}\in\Delta_t,\ \mathbf{x}_1=(z_1,0),\quad z_1\in\mathcal{G}_t, \tag{49}$$

where $\mathcal{G}_t$ is defined by Eqs. (40) and (44), and $F(\mathbf{x}_1,t)$ is given by Eq. (43). From Eqs. (46) and (49)

$$dG(\mathbf{x},t)=\Gamma(\mathbf{x},t)\Omega G(\mathbf{x},t), \tag{50}$$

$$G(\mathbf{x}_1,t)=F(\mathbf{x}_1,t). \tag{51}$$

By integrating Eq. (46) along the axis in a manner similar to that used to derive Eq. (43), we obtain

$$\mathfrak{F}(\mathbf{x}_2,\mathbf{x}_1,t)=F(\mathbf{x}_2,t)F(\mathbf{x}_1,t)^{-1}$$

if $\mathbf{x}_2=(z_2,0)$ and $z_2\in\mathcal{G}_t$. Therefore, from Eqs. (47), (49), and (51)

$$G(\mathbf{x},t)=\mathfrak{F}(\mathbf{x},\mathbf{x}_2,t)\mathfrak{F}(\mathbf{x}_2,\mathbf{x}_1,t)F(\mathbf{x}_1,t)$$

$$=\mathfrak{F}(\mathbf{x},\mathbf{x}_2,t)F(\mathbf{x}_2,t),$$

which shows that $G(\mathbf{x},t)$ as defined by Eq. (49) is independent of z_1.

Next, from Eqs. (48) and (49), and the fact that $F(\mathbf{x}_1,t)$ [as given by Eq. (43)] satisfies all of the Eqs. (17), we can show that $G(\mathbf{x},t)$ satisfies all of the Eqs. (17). In view of this result and Eqs. (50) and (51), we see that

$$F(\mathbf{x},t)=G(\mathbf{x},t).$$

The uniqueness of this solution is easily proven.

In summary, *for the values of t considered so far, we have established the existence of a unique solution* $F(t)$ *of Eqs.* (16), (17), *and* (43) *which is holomorphic over the domain* Δ_t.

(2) We next consider the values of t which we excluded in the first phase of the proof; i.e., we suppose that t is real and $-r_\Delta<z_t<0$. Then Δ_t is a union of two disjoint simply-connected regions $\Delta_t^{(1)}$ and $\Delta_t^{(2)}$ separated by the line K_t, and $\mathcal{G}_t$ is the union of two connected intervals $\mathcal{G}_t^{(1)}$ and $\mathcal{G}_t^{(2)}$ separated by the point z_t. We let $\mathfrak{F}^{(1)}(t)$ and $\mathfrak{F}^{(2)}(t)$ be defined in exactly the same way that the domain of $\mathfrak{F}(t)$ was defined above by Eqs. (46) except that the domain of $\mathfrak{F}^{(i)}(t)$ $(i=1,2)$ is $\Delta_t^{(i)}\times\Delta_t^{(i)}$, and we let

$$F^{(i)}(\mathbf{x},t):=\mathfrak{F}^{(i)}(\mathbf{x},\mathbf{x}_1,t)F(\mathbf{x}_1,t),$$

$$(\mathbf{x}_1=(z_1,0),\quad z_1\in\mathcal{G}_t^{(i)})$$

for all $\mathbf{x}$ in $\Delta_t^{(i)}$. Then the same method of proof which was used for the expression (49) can be used here to prove that $F^{(i)}(t)$ satisfies Eqs. (16), (17), and (43) and is holomorphic over its domain $\Delta_t^{(i)}$.

Next, let $F(t)$ be that function whose domain is Δ_t and which has the values

$$F(\mathbf{x},t)=F^{(i)}(\mathbf{x},t)$$

whenever $\mathbf{x}$ is in $\Delta_t^{(i)}$. Then, $F(t)$ *satisfies Eqs.* (16), (17), *and* (43) *and is holomorphic over* Δ_t. As before, uniqueness is easily proven.

(3) Next we consider any given point $\mathbf{x}$ in U_Δ, and we study the F-potential as a function of t over the domian $\Delta_\mathbf{x}$.

Any point t of $\Delta_\mathbf{x}$ is not a member of $K_\mathbf{x}$. Therefore, corresponding to each point t in $\Delta_\mathbf{x}$, the point $\mathbf{x}_t$ does not lie on the path $\mathbf{l}(\mathbf{x})$ which was defined by Eq. (38). Therefore, we may obtain the values $F(\mathbf{x},t)$ for all t in $\Delta_\mathbf{x}$ by integrating the ordinary differential equation corresponding to Eq. (16) along the path $\mathbf{l}(\mathbf{x})$ from its initial point $(-\xi,0)$ to its final point

$$\mathbf{x}=(z,\rho)=(Z(\xi,\eta),P(\xi,\eta)).$$

This differential equation is

$$\frac{\partial F(z',\rho',t)}{\partial\eta'}=-\frac{1}{2}\left(\frac{1}{r'_+-\tau}\frac{\partial r'_+}{\partial\eta'}+\frac{1}{r'_--\tau}\frac{\partial r'_-}{\partial\eta'}\right)\Omega F(z',\rho',t),$$

where it is to be understood that

$$z':=Z(\xi,\eta'),\quad \rho':=P(\xi,\eta'),$$

$$r'_\pm:=z'\pm i\rho',\quad 0\le\eta'\le\eta,$$

and where the initial value $F(-\xi,0,t)$ is given by Eq. (43).

Now, the factor of $F(z',\rho',t)$ on the right-hand side of the above differential equation is (for fixed ξ and η and for all η' such that $0\le\eta'\le\eta$) a holomorphic function of t over the domain $\Delta_{\mathbf{x}}$. Therefore, by a standard theorem, $F(\mathbf{x},t)$ *is, for fixed* $\mathbf{x}$, *a holomorphic function of* t *over the domain* $\Delta_{\mathbf{x}}$.

(4) In the first three steps of the proof we have shown that our F-potential is, for fixed t, a holomorphic function of $\mathbf{x}$ over the domain Δ_t; for fixed $\mathbf{x}$, the F-potential is a holomorphic function of t over the domain $\Delta_{\mathbf{x}}$. It follows from a theorem of Hartogs,[20] that F is a holomorphic function of (z,ρ,t) over the domian Δ.

(5) Finally, we consider the expression (45) for fixed $\mathbf{x}\ne(0,0)$. Since $t=\infty$ is a member of $\Delta_{\mathbf{x}}$ when $\mathbf{x}\ne(0,0)$, the expression (45) is holomorphic at $t=\infty$. Moreover, the determinant of (45) is, from Eqs. (17) and (20),

$$-t\lambda(t)^{-1}=-\tfrac{1}{2}[(z-\tau)^2+\rho^2]^{-1/2},$$

where $\tau=(2t)^{-1}$. Therefore, (45) has an inverse at $t=\infty$.

That completes our sketch of the proof of Theorem 2. *We let* $\mathcal{G}_0$ *denote the set of all potentials* F *for members of* V_0 *such that the domain* Δ *of* F *is in* $\mathfrak{D}_0$ *and such that the values of* $F(z,0,t)$ *over the domain* $\mathcal{J}$ *defined by Eq.* (40) *are given by Eq.* (43). In Sec. 5, we shall have occassion to consider other F-potentials for members of V_0, but all of them will be holomorphic continuations of members of $\mathcal{G}_0$; i.e., each of these F-potentials has a restriction to a domain which is in $\mathfrak{D}_0$ such that Eq. (43) holds for all (z,t) in $\mathcal{J}$.

E. Translations of z and τ

There remains one topic concerning the F-potential which we want to pursue here. In the treatment given above we selected the arbitrary constant in z so that $z_0=0$, where $(z_0,0)$ was a given point on the axis which was a member of U and which remained fixed throughout our discussion. This choice of the arbitrary constant in z helped to simplify our presentation. However, it is sometimes desirable to choose the arbitrary constant in z so that $z=\rho=0$ for some other point on the axis, which may not even be a member of U. Therefore, we shall now supply the transformation of the F-potential corresponding to the transformation

$$z\to z'=z+c,\quad \tau\to\tau'=\tau+c, \tag{52}$$

where c is any real constant, and this will enable the reader to extend all preceding results and later results involving F-potentials of members of V_0 to any value of z_0 which he prefers. The transformed F-potential is given by

$$F'(z',\rho,t')=F(z,\rho,t)\begin{pmatrix}1+2ct & 0\\ 0 & 1\end{pmatrix}. \tag{53}$$

The parameter t must be transformed simultaneously with the coordinate z as in Eq. (52) to leave

$$(2t)^{-1}\lambda(t)=[(z-\tau)^2+\rho^2]^{1/2}$$

invariant in value under the substitutions $z\to z'$, $t\to t'$. It is easily verified that $F'(z',\rho,t')$ satisfies all of the Eqs. (16), (17), and (43) over the transformed domain Δ' with (z,ρ,t) replaced by (z',ρ,t') in these equations. Note that the transformation (52) leaves the origin of the t plane invariant.

4. THE REPRESENTATION OF K

We employ a family of representations K_L of the Geroch group, one for each smooth contour L surrounding the origin in the complex plane and symmetric with respect to the real axis. K_L is the set of all holomorphic 2×2 complex matrix functions u such that the domain of u is a subregion of C, such that, for all t in this domain,[21]

$$u(t)^\dagger\epsilon u(t)=\epsilon,\quad \det u(t)=1,$$

$$u(t)^\dagger:=\text{h. c. of } u(t^*), \tag{54}$$

and such that L is contained in the domain of u, and

$$\begin{pmatrix}t^{-1} & 0\\ 0 & 1\end{pmatrix}u(t)\begin{pmatrix}t & 0\\ 0 & 1\end{pmatrix}\text{ is holomorphic at } t=\infty. \tag{55}$$

The subgroup K_0 of K which was mentioned in Sec. 1 and which transforms Minkowski space into the static Weyl space-times in V_0 is represented by the set K_{L0} of all diagonal members of K_L. The subgroup K_1 which contains the elements used by Hoenselaers, Kinnersley, and Xanthopoulos[11] to transform asymptotically-flat static Weyl space-times into asymptotically-flat members of V_0 is represented by the set K_{L1} of all matrices of the form

$$u^{(1)}(t)=\begin{pmatrix}1 & t\alpha(t)\\ 0 & 1\end{pmatrix},$$

where $\alpha(t)$ is holomorphic on L and at $t=\infty$; (only certain choices of $\alpha(t)$ yield asymptotically-flat results).

Any restriction on the gauge of the F-potentials results in a corresponding restriction on K_L. For example, Eq. (55) was derived from the gauge condition (24), which we always use. To derive the effect of any gauge restriction on K_L, we shall use the homogeneous Hilbert problem[7,22] (HHP) which was discussed in II and which furnishes our representation of a K-C transformation. Corresponding to each given F-potential $F^{(0)}$, each contour L such that $F^{(0)}$ has no fixed (independent of $\mathbf{x}$) t plane singularities in the region L_+ which is inside L, and each member u of K_L, a transformation

$F^{(0)}\to F$
(*always restricted to points* $\mathbf{x}$ *such that* $t(\mathbf{x})$, $t(\mathbf{x})^*$, *and the cut which joins them fall in the region* L_- *which is outside* L)

is determined from that solution (F,X_-) of the HHP,

$$X_-(t) = F(t)u(t)[F^{(0)}(t)]^{-1}, \tag{56}$$

for which[23] $F(t)$ is holomorphic at all points of $L + L_+$, $X_-(t)$ is holomorphic at all points of $L + L_-$ including $t = \infty$, and

$$F(0) = i\epsilon .$$

In II, Eq. (56) was given for all t on L; here, Eq. (56) will represent a holomorphic continuation of that equation into the entire complex plane minus those points of L_+ at which $u(t)$ has singularities or branch cuts. In II, we proved that if

(1) a solution of Eq. (56) subject to the stated conditions exists,

(2) dF has the same domain of holomorphy in the t plane as F itself, then the solution is unique, and F is the F-potential of a member of V. We shall deal with questions of existence in Sec. 5; until then we shall assume that the above two existence conditions are satisfied.

With the aid of the above HHP, it is clear that, if $F^{(0)}(t)$ satisfies the conditions given by Eq. (24), then $F(t)$ satisfies the same condition if and only if Eq. (55) holds. To help us discuss the effect of a much stronger gauge restriction on K_L, let

V_1 = set of all members of V for which F can be chosen so that its only t plane singularities are the ones at $t(\mathbf{x})$ and $t(\mathbf{x})^*$.

In Sec. 3, we proved that V_0 is a subset of V_1. It may be that V_1 is identical with V, but we have not been able to prove that as yet, and we would welcome a proof or a counterexample. In any case, it is clear from Eq. (56) that the following theorem holds.

Theorem 3: Let $\mathcal{G}_1$ *denote the set of all F-potentials of members of* V_1 *such that the only t plane singularities of each member of* $\mathcal{G}_1$ *are the ones at* $t(\mathbf{x})$ *and* $t(\mathbf{x})^*$ (so that each $\mathbf{x}$ section of the domain of F is the complex plane minus the points $t(\mathbf{x})$ and $t(\mathbf{x})^*$ and minus a cut which joins these points). *If* $F^{(0)}$ *is a member of* $\mathcal{G}_1$, *then F is a member of* $\mathcal{G}_1$ *if and only if*

$$\begin{pmatrix} t^{-1} & 0 \\ 0 & 1 \end{pmatrix} u(t) \begin{pmatrix} t & 0 \\ 0 & 1 \end{pmatrix} \tag{57}$$

is holomorphic on $L + L_-$ *including* $t = \infty$.

We shall let

$\mathcal{K}_L$:= *the set of all u in* K_L *such that the expression (57) is holomorphic throughout* $L + L_-$.

We shall be using the gauge $\mathcal{G}_1$ for all members of V_0 in this paper. Therefore, since we shall be primarily (though not exclusively) concerned with transformations of V_0 into V_0, we shall be using the subgroup $\mathcal{K}_L$ of K_L in almost all of our work. Note that $\mathcal{G}_0 \subset \mathcal{G}_1$.

At this point it is wise to give a precise understanding of the domain of the function F which is obtained from the solution of the HHP given by (56). Let

$\Delta^{(0)} := \operatorname{dom} F^{(0)}$,

$U_\Delta^{(0)}$:= set of all $\mathbf{x}$ in R_+^2 such that $(\mathbf{x}, t) \in \Delta^{(0)}$ for at least one $t \in C$, (58)

Δ_L := set of all $\mathbf{x}$ in $U_\Delta^{(0)}$ such that $F^{(0)}(\mathbf{x}, t)$ is holomorphic at all t in $L + L_+$ and such that our HHP has a solution [which satisfies the auxiliary conditions as well as Eq. (56)], (59)

$$\Delta := \{(\mathbf{x}, t) : \mathbf{x} \in \Delta_L,\ t \in (L + L_+) \cup (L_- \cap \Delta_{\mathbf{x}}^{(0)} \cap \operatorname{dom} u)\}. \tag{60}$$

It is clear that Δ is the domain of F. In the important special case when $u \in \mathcal{K}_L$, this domain Δ is simply the set of all $(\mathbf{x}, t)$ in $\Delta^{(0)}$ such that $\mathbf{x} \in \Delta_L$.

The HHP of Eq. (56) has many useful equivalent formulations. Perhaps the most obvious of these is the integral equation

$$\frac{1}{2\pi i} \int_L ds \frac{F(s)u(s)[F^{(0)}(s)]^{-1}}{s(s-t)} = 0, \quad (t \in L_+,\ \mathbf{x} \in \Delta_L) \tag{61}$$

subject to the conditions that $F(t)$ *be holomorphic in* $L + L_+$ *and satisfy*

$$F(0) = i\epsilon .$$

Equation (61) is an alternative form of the integral equation which was introduced and discussed[6] in I. Equation (61) taken together with the auxiliary conditions satisfied by F is easily shown to be equivalent to the Fredholm equation of the second kind

$$F(t) - \frac{1}{2\pi i} \int_L ds\, F(s)K(s,t) = F^{(0)}(t) \quad (t \in L,\ \mathbf{x} \in \Delta_L), \tag{62}$$

where

$$K(s,t) := \frac{t}{s(s-t)} [M(s,t) - u(s)M(s,t)u(t)^{-1}],$$

$$M(s,t) := F^{(0)}(s)^{-1}F^{(0)}(t), \tag{63}$$

and where $F(t)$ *is subject to the condition that it be holomorphic on L.* [Continuity on L is sufficient, since the existence of a holomorphic continuation on L is then implied by Eqs. (62) and (63).]

To aid our use of the Fredholm equation we shall now introduce a few conventional formal devices. Consider the set $C(L, 1, 2)$ of all 1×2 matrices $\psi(t)$ which are continuous functions of t on L, and define

$$\|\psi\| := \max_{t\in L}\{|\psi_1(t)|, |\psi_2(t)|\}.$$

The set $C(L,1,2)$ taken together with the above definition of a *norm* for its members is a Banach space. For any continuous 2×2 matrix function A whose domain is $L \times L$, we define $\psi\cdot A$ as that function whose domain is L and which has the values

$$(\psi\cdot A)(t) := \frac{1}{2\pi i}\int_L ds\, \psi(s)A(s,t).$$

Thus, A plays the role of a linear operator (a completely continuous one) on the Banach space. Its *norm* $\|A\|$ is defined as the least upper bound of the set

$$\{\|\psi\|^{-1}\|\psi\cdot A\| : \psi \in C(L,1,2),\ \psi \neq 0\}.$$

In terms of these notations, Eq. (62) is expressible in the form

$$F(\mathbf{x})\cdot[I - K(\mathbf{x})] = F^{(0)}(\mathbf{x}), \tag{64}$$

where we have, with future applications in mind, chosen to make the dependence on $\mathbf{x}$ explicit. $F^{(0)}(\mathbf{x})$ denotes that function whose domain is $\Delta_{\mathbf{x}}^{(0)}$ and whose values are $F^{(0)}(\mathbf{x}, t)$. Each row of $F^{(0)}(\mathbf{x})$ is a member of $C(L, 1, 2)$ with its own norm.

5. THE GEROCH CONJECTURE

We shall now use the Fredholm equation to prove the second of the two existence conditions which were mentioned earlier in Sec. 4 and which were assumed[7] without proof in II. In fact, the following theorem goes beyond that existence condition and asserts that the solution F which is obtained from our HHP or from any of the equivalent integral equations is a holomorphic function of (z, ρ) as well as of t.

Theorem 4: *Let* $U_\Delta^{(0)}$, Δ_L, *and* Δ *be defined by Eqs.* (58)–(60).

(a) *Suppose* $\mathbf{x} \in U_\Delta^{(0)}$ *such that* $F^{(0)}(\mathbf{x})$ *is holomorphic at all* t *in* $L + L$. *Then a solution of Eq.* (62) *exists*, (i.e., $\mathbf{x} \in \Delta_L$) *if and only if* $I - K(\mathbf{x})$ *has an inverse as a linear operator on the Banach space* $C(L, 1, 2)$.

(b) Δ_L *and* Δ *are open subsets of* R_+^2 *and of* $R_+^2 \times C$, *respectively.*

(c) F *is holomorphic at all* $(\mathbf{x}, t)$ *in* Δ.

We shall give the proof of the above theorem in three parts. The first part proves statement (a) of the theorem.

(1) Let $\mathbf{x} \in U_\Delta^{(0)}$ such that $F^{(0)}(\mathbf{x})$ is holomorphic in $L + L_+$. If $[I - K(\mathbf{x})]^{-1}$ exists, the solution

$$F(\mathbf{x}) = F^{(0)}(\mathbf{x}) \cdot [I - K(\mathbf{x})]^{-1}$$

exists and is unique, virtually by definition of the inverse.

Conversely, suppose a solution $F(\mathbf{x})$ exists. *Then it is unique, since the solution* (for given $\mathbf{x}$) *of our* HHP *is unique if it exists.* For suppose, for given $\mathbf{x}$, that (F, X_-) and (F', X_-') are both solutions of Eq. (56). Then (suppressing $\mathbf{x}$)

$$F' F^{-1} = X_-' X_-^{-1} .$$

Therefore $F' F^{-1}$ is an entire function of t and is holomorphic at $t = \infty$. Therefore, $F' F^{-1}$ is t-independent. However, $F(0) = F'(0) = i\epsilon$. So, $F' = F$ for all t.

Moreover, if $F(\mathbf{x})$ exists, $[I - K(\mathbf{x})]^{-1}$ exists since, otherwise, the solution would not be unique, and we would have a contradiction. To see this, note that the nonexistence of the inverse implies the existence of a nonzero member $\psi(\mathbf{x})$ of $C(L, 1, 2)$ such that

$$\psi(\mathbf{x}) \cdot [I - K(\mathbf{x})] = 0 ,$$

whereupon

$$F(\mathbf{x}) + \begin{Bmatrix} \psi(\mathbf{x}) \\ \psi(\mathbf{x}) \end{Bmatrix}$$

would also be a solution of Eq. (64).

We next prove statement (b) of the theorem.

(2) Let $\mathbf{x}_1$ be any member of Δ_L. From the preceding part of the proof, $I - K(\mathbf{x}_1)$ has an inverse. Since I and $K(\mathbf{x}_1)$ are bounded linear operators and, since $I \neq K(\mathbf{x}_1)$,

$$\infty > \delta := \| (I - K(\mathbf{x}_1))^{-1} \|^{-1} > 0 . \tag{65}$$

There then exists a neighborhood $N(\mathbf{x}_1) \subset U_\Delta^{(0)}$ of the point $\mathbf{x}_1$ such that, for all $\mathbf{x}$ in $N(\mathbf{x}_1)$, $F^{(0)}(\mathbf{x})$ is holomorphic at all t in $L + L_+$, and

$$\| K(\mathbf{x}) - K(\mathbf{x}_1) \| < \delta . \tag{66}$$

[To see this, recall that, by choice of L, all fixed singularities and cuts of $F^{(0)}(\mathbf{x})$ are in L_-; by definition of Δ_L, $t(\mathbf{x}_1)$, $t(\mathbf{x}_1)^*$, and the cut which joins them are also in L_-. Since the cut which joins $t(\mathbf{x})$ to $t(\mathbf{x})^*$ *is always chosen*[24] *so that it varies smoothly with* $\mathbf{x}$ and since $K(\mathbf{x})$ is a continuous function of $\mathbf{x}$ in the strong convergence sense, the existence of $N(\mathbf{x}_1)$ follows.]

Now, for all $\mathbf{x}$ in $N(\mathbf{x}_1)$,

$$I - K(\mathbf{x}) = [I - K(\mathbf{x}_1)] \cdot \{ I - [I - K(\mathbf{x}_1)]^{-1} \cdot [K(\mathbf{x}) - K(\mathbf{x}_1)] \} . \tag{67}$$

Since

$$\| [I - K(\mathbf{x}_1)]^{-1} \cdot [K(\mathbf{x}) - K(\mathbf{x}_1)] \| < 1 , \tag{68}$$

it follows that $I - K(\mathbf{x})$ has an inverse for all $\mathbf{x} \in N(\mathbf{x}_1)$. So, $N(\mathbf{x}_1) \subset \Delta_L$ for any choice of $\mathbf{x}_1 \in \Delta_L$.

Therefore, Δ_L is an open subset of R_+^2.

That Δ is an open subset of $R_+^2 \times C$ follows from the facts that Δ_L is an open subset of R_+^2, and

$$(L \cup L_+) \cup (L_- \cap \Delta_{\mathbf{x}}^{(0)} \cap \operatorname{dom} u)$$

is an open subset of C. We leave details to the reader.

(3) To prove the holomorphy of F, we first replace $F^{(0)}$ by its holomorphic extension $[F^{(0)}]$ to a region $[\Delta^{(0)}]$ in $C \times C \times C$. All preceding arguments remain valid [though $t(\mathbf{x})^*$ now means the complex conjugate of $t(\mathbf{x}^*)$] for complex $\mathbf{x}_1$ and $\mathbf{x}$. Equations (64)–(68) still hold; so, for $\mathbf{x} \in N(\mathbf{x}_1)$,

$$F(\mathbf{x}) = F^{(0)}(\mathbf{x}) \cdot [I + T(\mathbf{x}) + T(\mathbf{x})^2 + \cdots] \cdot [I - K(\mathbf{x}_1)]^{-1} ,$$

where

$$T(\mathbf{x}) := [I - K(\mathbf{x}_1)]^{-1} \cdot [K(\mathbf{x}) - K(\mathbf{x}_1)] ,$$

$$T(\mathbf{x})^n := T(\mathbf{x})^{n-1} \cdot T(\mathbf{x}) .$$

For fixed $t \in L$, each term in the above Neumann series expansion is a holomorphic function of $\mathbf{x}$ at all points of Δ_L. However, the series converges uniformly with respect to $\mathbf{x} \in N(\mathbf{x}_1)$. Therefore, $F(\mathbf{x}, t)$ is, for fixed $t \in L$, a holomorphic function of $\mathbf{x}$ at all points of $N(\mathbf{x}_1)$. Since $\mathbf{x}_1$ is an arbitrary point in Δ_L, we obtain the following statement.

(A) If $t \in L$, $F(\mathbf{x}, t)$ is a holomorphic function of $\mathbf{x}$ at all points of Δ_L.

To extend the above statement to other values of t, we note that Eq. (56) implies, for all $\mathbf{x} \in \Delta_L$,

$$F(t) = \frac{1}{2\pi i} \int_L ds \, \frac{F(s)}{s - t} \quad (t \in L_+) ,$$

$$F(t) = \frac{-t}{2\pi i} \int_L ds \, \frac{F(s) u(s) F^{(0)}(s)^{-1} F^{(0)}(t) u(t)^{-1}}{s(s - t)}$$

$$(t \in L_-) .$$

Therefore, the preceding conclusion (A) can be generalized as follows:

(B) If $t \in C$, then $F(t)$ is a holomorphic function of x at all points of $\Delta_t := \{\mathbf{x} \in \Delta_L : (\mathbf{x}, t) \in \Delta\}$, a set which is identical to Δ_L for $t \in L + L_+$, but a nonempty proper subset of Δ_L for $t \in L_- \cap \operatorname{dom} u$.

We next consider fixed $\mathbf{x}\in\Delta_L$. By definition of our HHP $F(\mathbf{x})$ is holomorphic at all t in $L+L_+$. Also, from Eq. (56),

$$F(t)=X_-(t)F^{(0)}(t)u(t)^{-1}.$$

Therefore, $F(\mathbf{x})$ is also holomorphic at all t in

$$L_-\cap\Delta_{\mathbf{x}}^{(0)}\cap \operatorname{dom} u .$$

In other words, we have the following conclusion:

(C) If $\mathbf{x}\in\Delta_L$, $F(\mathbf{x},t)$ is a holomorphic function of t at all points of $\Delta_{\mathbf{x}}:=\{t\in C:(\mathbf{x},t)\in\Delta\}$.

From (B) and (C), we conclude that F is holomorphic.[20] *That completes our proof.*

The above theorem leaves two questions unanswered. First, is Δ connected? (If Δ is not connected, it may still be possible to deform L outward without crossing any singularities of u in such a way that the new Δ is connected.) We have not yet found a way of handling this question.

Second, and more crucial, does F exist? In other words, is Δ_L not empty? We do not have an answer to this question for arbitrary $F^{(0)}$ and u. However, we do have an answer for the case which "really counts."

Theorem 5: *Suppose $F^{(0)}\in\mathcal{G}_0$ or is a holomorphic continuation of a member of $\mathcal{G}_0$, and $u\in\mathcal{K}_L$.*

(a) *There exists an open interval I_L of the axis such that*

$$(0,0)\in I_L\subset\Delta_L .$$

(b) *For all $(z,0)$ on I_L, $\mathcal{E}(z,0)$ is given by* Eq. (1), *and $F(z,0,t)$ is given by Eq.* (43).

(c) *F is a holomorphic continuation of at least one member of $\mathcal{G}_0$; in particular, therefore, F is an F-potential for a member of V_0.*

The proof will be given in three parts. In the proof, we use the notations $\Delta^{(0)}$, $U_\Delta^{(0)}$, Δ_L, and Δ, which are defined by Eqs. (58) to (60).

(1) We recall that, if $t\neq\infty$, then $(0,0,t)\in\Delta^{(0)}$. Since $L+L_+$ is a bounded set, $(0,0,t)\in\Delta^{(0)}$ for every t in $L+L_+$; moreover, there must exist an open subset

$$N(0,0)\subset U_\Delta^{(0)}$$

such that $(0,0)\in N(0,0)$, and

$$N(0,0)\times(L+L_+)\subset\Delta^{(0)} .$$

Note that the set of all $(z,0)$ in $N(0,0)$ is a union of one or more disjoint open intervals of the axis. Let I_L be that one of the open intervals which covers $(0,0)$. Then $(z,0,t)\in\Delta^{(0)}$ for every $(z,0)\in I_L$ and $t\in(L+L_+)$; so $F^{(0)}(z,0,t)$ is, if $(z,0)\in I_L$, a holomorphic function of t throughout $L+L_+$.

At this point we request the reader to review Sec. 3C. It can be seen that, if $t\in(L+L_+)$, then $F^{(0)}(z,0,t)$ is given by Eq. (43), with the $\mathcal{E}$-potential on the axis given by $\mathcal{E}^{(0)}(z,0)$. This result is obtained by integrating the first of Eqs. (41) along I_L, with $F^{(0)}(0,0,t)$ *defined* by Eq. (43).

(2) The next step in our proof is to show that $I_L\subset\Delta_L$, which will be done once we show that our HHP has a solution for every $(z,0)\in I_L$.

We shall consider the expression (43) as a possible solution of Eq. (61) (which is equivalent to the HHP for points $(z,0)\in I_L$. Upon substituting from Eq. (43) into Eq. (61) (for both $F^{(0)}$ and F) we find that the integral over s can be computed easily, with the result that the *left-hand side* of Eq. (61) has all of its matrix elements vanishing except for the (4, 3) element, which equals

$$(1-2tz)^{-1}[i\mathcal{E}^{(0)}(z,0)u_3^3(k)-k^{-1}u_4^3(k)$$
$$-k\mathcal{E}(z,0)\mathcal{E}^{(0)}(z,0)u_3^4(k)-i\mathcal{E}(z,0)u_4^4(k)],$$

where $k=(2z)^{-1}$. *So* Eq. (43) *supplies us with a solution of* Eq. (61) *if and only if the above expression vanishes*, i.e., *if and only if $\mathcal{E}(z,0)$ is given by* Eq. (1) *when* $(z,0)\in I_L$. So, $I_L\subset\Delta_L$.

(3) That the solution F is the F-potential of a member of V_0 follows since $\mathcal{E}=\dot{F}_{44}(0)$ is holomorphic in a neighborhood of a point $(0,0)$ of the axis. That F is an extension of a member of $\mathcal{G}_0$ can be seen by restricting F to a domain such as the one defined by Eqs. (25)–(30), *with r_Δ chosen sufficiently small.*

That completes our proof of Theorem 5. We are at last in a position to prove the Geroch conjecture in the form given by the *first sentence* of Theorem 1 in Sec. 1. Note that part (c) of Theorem 5 already contains the second sentence of Theorem 1 as a special case, i.e., *any element of $\mathcal{K}_L$ transforms Minkowski space* (MS) *into a member of V_0*. It remains to prove the first sentence in Theorem 1, i.e., *any given member of V_0 can be obtained from* MS *by the* K-C *transformation corresponding to at least one element of $\mathcal{K}_L$*.

Proof of Geroch conjecture: Consider any given member of V_0, say

$$S_g:=S_{\text{given}}$$

with an $\mathcal{E}$-potential $\mathcal{E}_g$ whose domain is U_g. By definition of V_0, U_g contains at least one point $(z_0,0)$ of the axis; we follow our usual practice of selecting the arbitrary constant in z so that $z_0=0$. Observe that there exists at least one 2×2 matrix function $u(t)$ of a complex variable t such that the domain of u is a neighborhood of ∞, and

$$\det u(t)=1,\quad u(t)^\dagger\epsilon\, u(t)=\epsilon,$$
$$\mathcal{E}_g(\tau,0)[t\,u_3^4(t)+iu_4^4(t)]+t^{-1}u_4^3(t)-iu_3^3(t)=0, \tag{69}$$

where $\tau=(2t)^{-1}$. An example would be[25]

$$u(t)=\begin{pmatrix}\exp[-\xi(t)] & t\alpha(t)\cdot\exp[\xi(t)]\\ 0 & \exp[\xi(t)]\end{pmatrix},$$

where

$$\exp[-2\xi(t)]+i\alpha(t)=\mathcal{E}_g(\tau,0).$$

Select a maximal holomorphic continuation of a $u(t)$ which satisfies Eqs. (69). Then it can be seen that there exists at least one contour L such that $u\in\mathcal{K}_L$.

We next consider the K-C transformation corresponding to the above choices of u and L and to

$F^{(0)}=$ the F-potential for Minkowski space,[2,7]

$\mathcal{E}^{(0)}=1=$ the $\mathcal{E}$-potential for Minkowski space.

According to Theorem 5, a unique solution F of the HHP or of any of the equivalent integral equations exists and is an F-potential for a member S of V_0; moreover, F is an extension of at least one member of $\mathcal{G}_0$, and $\mathcal{E}$ and u are related by Eq. (1) with $\mathcal{E}^{(0)}=1$. *To prove the*

Geroch conjecture, i.e., *Theorem* 1, *it is sufficient to prove that* $S=S_g$, *and we shall now do this.*

Since $\mathcal{E}^{(0)}=1$ at all points of R^2_+, Eqs. (1) and (69) imply

$$\mathcal{E}_g(z,0)=\mathcal{E}(z,0) \tag{70}$$

for all $(z,0)$ in at least one open interval J of the axis such that $(0,0)\in J$. From Eqs. (10) and (70), we prove that

$$\left[\frac{\partial^{m+n}\mathcal{E}_g(z,\rho)}{\partial z^m\partial\rho^n}\right]_{\rho=0}=\left[\frac{\partial^{m+n}\mathcal{E}(z,\rho)}{\partial z^m\partial\rho^n}\right]_{\rho=0},$$

$$m\geq 0,\quad n\geq 0,$$

for all $(z,0)\in J$. Therefore, since $\mathcal{E}$ and $\mathcal{E}_g$ are holomorphic,

$$\mathcal{E}_g(z,\rho)=\mathcal{E}(z,\rho)$$

at all points (z,ρ) in at least one neighborhood of $(0,0)$. Therefore, $\mathcal{E}_g$ and $\mathcal{E}$ have a common extension. So S_g is the same space-time as S; *the Geroch conjecture is proved.*

6. DISCUSSION AND PERSPECTIVES

Since Sec. 1, we have considered only those $\mathcal{E}$-potentials which are defined over a domain in which $f>0$, i.e., one of two Killing vectors characterizing the space-time is timelike. It is true that many of our equations are valid as they stand for the other case, where $f<0$. Examples of equations which are valid for both cases are the homogeneous Hilbert problem and integral equations in Eqs. (56)–(63).

However, in general, the equations which we have given do not apply when both Killing vectors are spacelike, i.e., $f<0$. This presents no severe problem. To obtain the correct *form* of the negative *f equations* from the positive *f equations*, and vice versa, all we have to do is make the formal replacements

$$z\to z,\qquad \rho\to i\rho,$$

$$\partial/\partial z\to\partial/\partial z,\quad \partial/\partial\rho\to -i\partial/\partial\rho, \tag{71}$$

whenever z, ρ, $\partial/\partial z$ and $\partial/\partial\rho$ appear in any of the equations given *in this paper*. (In II,[7] an additional substitution $*\to i*$, where $*$ is a two-dimensional duality operator, was required.)

The above rule (71) will furnish the correct *forms* of the equations, but it does not transform *given* solutions of these equations. To transform a solution for the F-potential corresponding to positive f to a solution corresponding to negative f, we could use the substitution

$$F_+(z,\rho,t)\to F_-(z,\rho,t)=F_+(z,i\rho,t),$$

with like rules for h, $\mathcal{E}$, H, etc. However, this rule also changes the spacetime signature. For example, we use a signature $+++-$ as in Eq. (4), and the above rule combined with (71) would switch us to $+---$ [since $h(z,i\rho)$ has a signature $--$ if $h(z,\rho)$ has a signature $++$]. To preserve the signature, the correct substitution is

$$F_-(z,\rho,t)=-[F_+(z,i\rho,t)]^*, \tag{72}$$

where * means "take the complex conjugate of $F_+(z^*,-i\rho^*,t^*)$" (i.e., the * operation does not destroy the holomorphy of the function). The same rule applies to h, $\mathcal{E}$, H, etc.

The above formal rules (71) and (72) do not, however, take care of all questions concerning the negative f potentials. There remains the problem of the domain of these potentials. It would be useful for someone to give, for negative f, a precise description of the set of domains $\mathfrak{D}_0$ which we defined in Sec. 3.

In fact, whether $f>0$ or $f<0$, it would be desirable to make a deep study of the domains of holomorphy of the F-potentials. In doing this, we feel that the "natural domains" of the F-potentials (and, also, of $\mathcal{E}$ and H) should be the domains of their holomorphic continuations (or even of multiple values analytic continuations) involving complex z and ρ. At the present time, we are a long way from having anything but a casual working knowledge of F-potential domains in the extended sense of the term. In II, some attempts in the direction of a deeper understanding were made.[7]

There are at least three important problems whose handling would be facilitated by a better understanding of the domains and of the holomorphic continuations (and, we may add, of the singularities) of F-potentials. The first of these problems resolves around the following question:

(1) *Are there any members of V which are not in V_0 and which can be generated from* MS *by a $u(t)$ which is not in $\mathcal{K}_L$?*

To answer this question it is important to know (for example) whether the gauge of the F-potentials for such members of V can be restricted to $\mathcal{G}_1$. (See Theorem 3 in Sec. 4 for the definition of $\mathcal{G}_1$.) In a few special cases, we have found that this can be done, but we have no generally applicable conclusion. Though the problem may appear not to be an exciting one to the reader, we cannot say that our understanding of the Geroch group is thorough as long as the problem of SAV's which are not in V_0 remains unresolved.

A second and more physically satisfying problem is furnished by the following question:

(2) *Corresponding to that $F^{(0)}$ which is the F-potential for* MS *and to any given $u(t)$ in $\mathcal{K}_L$, precisely what are the relations between the analytical properties* (especially the singularities in L_+) *of $u(t)$ and various interesting points in the space-time corresponding to F or on the boundary of that space-time* (e.g., singularities and horizons)?

A thorough analysis which would lead to some interesting answers to the above question would be welcomed by all.

Finally, there is a third problem which can best be described after a few introductory remarks. Consider the restrictions of all F-potentials for members of V_0 to the gauge $\mathcal{G}_0$. Thus, any solution for F which is obtained as a result of a K-C transformation involving an $F^{(0)}$ in $\mathcal{G}_0$ and a u in $\mathcal{K}_L$ is automatically to be restricted so that it becomes a member of $\mathcal{G}_0$. (This can always be done according to Theorem 5.) Moreover, let any two members of $\mathcal{G}_0$ be regarded as equal if they are equal in at least one neighborhood of the point $(0,0,0)$. *Then, with these conventions understood, the family of* K-C *transformations of $\mathcal{G}_0$ into $\mathcal{G}_0$ is a group.*

However, that kind of formal construction of a group should not blind us to a potentially interesting problem. What about the "full" solution for F as opposed to its restriction to a member of $\mathcal{G}_0$?

(3) *Are there domains of the $\mathcal{E}$-potentials of some full solutions of the* HHP *which are not connected, which cannot be made connected by analytic continuation in the real (z,ρ)-manifold, and whose various connected components correspond to different space-times in V?*

As yet, we have not been able to *eliminate* such possibilities *except in special cases.*

In answering the above question and others, a great help may be offered by the fact that any $u(t)$ can be factored into a product involving only a few factors of the form

$$u^{(1)}(t)=\begin{pmatrix}1 & t\alpha(t)\\ 0 & 1\end{pmatrix} \text{ or } j(t):=\begin{pmatrix}0 & -t\\ t^{-1} & 0\end{pmatrix}.$$

The elements $u^{(1)}$ constitute that subgroup K_1 of the Geroch group which was discussed in Sec. 1. The element $j(t)$ of $\mathcal{K}_L$ induces the transformation

$$\epsilon\rightarrow\epsilon^{-1},$$

and the corresponding transformation of the F-potential is easily computed.

As regards $u^{(1)}$, the authors have derived a regular nonmatrix Fredholm equation of the second kind which can be used to effect K-C transformations induced by $u^{(1)}$ for arbitrary $F^{(0)}$. The massive theoretical and practical knowledge concerning this kind of Fredholm equation makes it a powerful analytical tool, especially when it is used in conjunction with Eq. (1).

Equation (1) *also makes it a trivial matter to find a suitable*[26] *$u(t)$ which transforms any given member of V_0 into any other given member of V_0.* For example, we have used it to find a $u(t)$ which transforms MS into Kerr[27]; it can be used similarly to find a $u(t)$ which transforms MS into any Tomimatsu–Sato solution, including all known generalizations of the T–S solutions. In a subsequent paper the derivation of the T–S solutions will be given as an illustrative example of the use of our Fredholm equation.

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[13]Equation (1) holds in a neighborhood of $z=0$. [We have chosen the arbitrary constant in z so that $(0,0)\in U$.] To obtain the family of all $u(t)$ corresponding to given $\mathcal{E}^{(0)}(z,0)$ and $\mathcal{E}(z,0)$, we replace k by t, which supplies $u(t)$ in a neighborhood of $t=\infty$; then, we conduct a maximal holomorphic continuation of $u(t)$.

[14]F. J. Ernst, J. Math. Phys. **15**, 1409 (1974). The potential ξ in this paper is related to $\mathcal{E}$ by $\mathcal{E}=(\xi-1)(\xi+1)^{-1}$.

[15]See, for example, Theorem 3 in Chap. II of *Several Complex Variables* by S. Bochner and W. T. Martin (Princeton U. P., Princeton, 1948).

[16]In. Ref. 7, we considered a domain which involved complex z and ρ. Here, we shall only consider complex z and ρ in some proofs concerning the holomorphy of F.

[17]In Ref. 7, we were not aware of this exceptional case and did not allow for it in our discussion and proofs. However, a simple modification of the proofs (e.g., as in the proof of Theorem 2 of the present paper) takes care of the problem.

[18]We caution the reader that, for given $\mathbf{x}$, the *full analytic continuation* of F (which is multiple-valued) can and generally does have t plane singularities at points other than $t(\mathbf{x})$ and $t(\mathbf{x})^*$; these singularities are independent of $\mathbf{x}$. (We feel that our discussion in Sec. 3 of Ref. 7 created or left room for a misconception concerning this very point. In the present paper, the problem does not even arise.)

[19]In Ref. 7, we defined $\mathcal{F}(\mathbf{x},\mathbf{y},t)$ for complex $\mathbf{x}$ and $\mathbf{y}$ over a multiply connected domain. The statement after Eq. (58) in Sec. 3 of Ref. 7 that the multiple-valued $\mathcal{F}$ has no singularities in $[U]\times[U]\times C$ except for the zeros of $\tau\lambda(\mathbf{x},t)$ and $\tau\lambda(\mathbf{y},t)$ is false. However, this statement was never used and led to no further errors.

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[21]Our definition of $u(t)$ has undergone some changes since the introduction of this concept in Ref. 6. In Ref. 6, we let $u(t):=\exp[\gamma(t)\epsilon]$ where $\gamma(t)$ is Hermitian for real t and is holomorphic in an annulus surrounding the origin. This definition was dropped in Ref. 7, because the set of functions $\exp(\gamma\epsilon)$ (as we defined them in Ref. 6) does not constitute a group; we had not considered this objection before Ref. 7. Also the gauge condition of Eq. (55) was added in Ref. 7, where questions concerning gauge were first discussed.

[22]As one of the applications of the HHP in Ref. 7, we obtained that general transformation of Minkowski space into a static Weyl vacuum space-time which is induced by any member of K_{LO}.

[23]The auxiliary conditions which must be satisfied by F and X_- can be given in a slightly weaker form, viz., it is sufficient to state that F is continuous in $L+L_+$ and is holomorphic in L_+, while X_- is continuous in $L+L_-$ and is holomorphic in L_-. However, the stronger additional conditions, which we given in this present paper, of holomorphy on L is then implied by the facts that $u(t)$ and $F^{(0)}$ are holomorphic on L. [In Ref. 7, we gave the additional conditions that F^{-1} exists for all t in $L+L_+$, and X_-^{-1} exists for all t in $L+L_-$. However, these are implied by the conditions given in the present paper; this can be seen by taking the determinant in Eq. (56) and noting that it is an entire function and is also holomorphic at $T=\infty$.]

[24]This is a point which we have stressed for the first time in the present paper. It is automatically implied for the set $\mathcal{D}_0$ of F-potential domains which we defined in Sec. 3.

[25]This example represents a transformation in K_O followed by a transformation in K_1 as described in Sec. 1 and used for special ξ and α) in Refs. 11 and 12. Observe that $\xi(t)$ and $\alpha(t)$ are real for real t.

[26]The group $\mathcal{K}$ is multiply transitive; i.e., the $u(t)$ which induces a transformation of any given member of V_0 into another given member of V_0 is not unique. For example, if u induces a transformation of F^{MS} into F, then so does $u u_B$ where u_B is any B-group member as defined by Eq. (14) in Ref. 7.

[27]This kind of phrasing uses poetic license. Actually, we are transforming F-potentials, and the F^{MS} which we are employing here is the one corresponding to the choice $\mathcal{E}^{MS}=1$. The same transformation applied to an F^{MS} for which $\mathcal{E}^{MS}=1+iq$ where q is a nonzero real parameter may yield a radically different result. An interesting example will be given in a forthcoming paper.

Nonglobal proof of the thin–sandwich conjecture

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A gravitational thin–sandwich conjecture was first proposed by Wheeler and coworkers during the period 1962–4. The present paper contains a proof of the nonglobal form of this gravitational thin–sandwich conjecture. The proof (a) applies for arbitrary choices of the spatial metric and its time derivative; and (b) demonstrates the existence on a spacelike three-surface of solutions which satisfy conditions of continuity known to be sufficient to obtain existence and uniqueness of solutions to Einstein's equations off the three-surface and existence and uniqueness of geodesics. Riquier's existence theorem plays an important role in the proof. The relationship of the present results to previous work is discussed. Some global questions associated with the thin–sandwich conjecture are clarified. Some aspects of the relationship of the thin–sandwich conjecture to the problem of the quantization of the gravitational field are noted. Both the vacuum case and the case of a nonviscous fluid are included. The discussion allows for an arbitrary equation of state $p = p(\rho)$.

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I. INTRODUCTORY REMARKS

The main result contained in the present paper is a proof of the nonglobal form of the thin–sandwich conjecture of general relativity. The results presented here provide the first internally self-consistent proof which (a) applies for arbitrary choices of the spatial metric and its time derivative and (b) demonstrates the existence on a spacelike three–surface of solutions which satisfy conditions of continuity known to be sufficient to obtain existence and uniqueness of solutions to Einstein's field equations off the three-surface. Another feature of the present paper not found in previous discussions of the case of arbitrary spatial metric and its time derivative is the inclusion of an explicit discussion of continuity.

The gravitational thin–sandwich problem is a special case of the gravitational initial value problem.[1] The present paper includes a discussion of the thin–sandwich problem in the case of a nonviscous gravitating fluid with arbitrary equation of state[1] $p = p(\rho)$ so as to allow for appliations of the discussion to objects such as supermassive stars[2] and neutron stars[3] in which general relativity is believed to play a major role.

The least restrictive continuity requirements on the N^i and N known to be sufficient to obtain existence and uniqueness of solutions to Einstein's field equations off the spacelike three–surface, and existence and uniqueness of geodesics have been given by Hawking and Ellis.[4] This existence and uniqueness theorem requires initial functions N, N^i and, γ_{ij} on the three–surface of class C^n, where it is necessary that one have $n \geqslant 2$ and sufficient if $n \geqslant 4$, and initial functions $\gamma_{ij,0}$ of class C^p where it is necessary that one have $p \geqslant 1$ and sufficient if $p \geqslant 3$. The interesting existence discussion of J. A. Wheeler[4] proves existence of N^i and N of class C^{1-}. The theorems of the present paper prove existence of functions N^i and N which are analytic (i.e., expandable in power series) and also are of class C^∞, since analyticity implies continuity of class C^∞.

Komar's first paper[5] on the thin–sandwich equations constitutes some progress toward a proof. The simplest way to distinguish between the present results and Komar's discussion is to note that the goal of Komar's discussion is to demonstrate existence for arbitrary choices of N, N^i, $N^1{}_{,3}$; and $N^2{}_{,3}$ on a two-surface $x^3 =$ const within the three-surface. Here Komar's notation and coordinate labeling has been converted to the notation and coordinate labeling of the present paper; the quantities N and N^i are the lapse and shift functions which are defined in detail in Sec. III of this paper. By comparison, the goal of the present discussion is to demonstrate existence and uniqueness for arbitrary choices of N and $N_{,3}$ and N^i, $N^1{}_{,3}$ on a two-surface $x^3 =$ const within the three-surface and arbitrary choices of $N^2{}_{,3}$ on a line within the three-surface. Note that N and N^i are distinct geometrical entities under coordinate transformations within the three-surface. N is a scalar and N^i a vector. Also note that the present paper includes a discussion of the nonvacuum case, whose significance is discussed at the end of Sec. IV and of Ref. 3.

P. G. Bergmann has noted some of the difficulties involved in proofs of the thin–sandwich conjecture.[6] It is suggested by the present author that these difficulties can best be thought of as presenting a problem in partial differential algebra[6] and can be usefully attacked by the use of Riquier's existence theorem.[6] The equations which must be considered in a proof of the gravitational thin–sandwich conjecture are both nonlinear and severely coupled. And it is in the analysis of such systems of equations that Riquier's existence theorem, by providing a detailed logical basis for one's algebraic manipulations, becomes well-nigh indispensable.

II. THE QUANTIZATION OF THE GRAVITATIONAL FIELD

Some authors have suggested that a proof of the thin–sandwich conjecture may be of help in the problem of the quantization of the gravitational field. (See P. G. Bergmann, Ref. 6.) This problem may be addressed using adaptations of

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the techniques of Tomonaga-Schwinger or of Feynman. The equivalence of the theory which underlies these two techniques has in the case of Lorentz–covariant quantum electrodynamics been demonstrated by Dyson.

It will be useful to mention here two pertinent aspects of the problem of quantizing the electromagnetic field which clarify the problem of quantizing the gravitational field. First there is the role played by gauge invariance[7–11] in quantum electrodynamics both from the Schwinger[7,9] and the Feynman[8] viewpoints. Second there is the role played by one or more initial-value equations as constraints[9] on the field variables of electrodynamics. The similarity between the gravitational and electromagnetic fields stems from the fact that the gravitational field, like the electromagnetic field, exhibits gauge invariance and also satisfies one or more equations of constraint.

In the present paper the general covariance in space time of Einstein's equations reveals itself as spatial covariance of the gravitational initial-value equations, which implies covariance of the initial-value equations under the infinitesimal spatial coordinate transformations $\bar{x}^i = x^i + \xi^i$ where $\xi^i(x^k)$ is an infinitesimal vector field. This coordinate transformation generates the gauge transformation $g_{ij} \to \bar{g}_{ij} + \xi_{i|j} + \xi_{j|i}$ in the g_{ij} and corresponding transformations in the other spatial tensors appearing in the initial value equations. (Note that $i, j = 1,2,3$.)

With these facts in mind, the results of Sec. IV of the present paper demonstrating that the 12 functions γ_{ij} and $\gamma_{ij,0}$ can be specified freely (i.e., chosen independently and arbitrarily) on a spacelike three–surface can be compared with the thin–sandwich theorem of electromagnetism which shows that the six functions A_i and $A_{i,0}$ can be specified freely on a spacelike three-surface. (See J. A. Wheeler, Ref. 4, p. 245, Eq. (36) to obtain the electromagnetic thin–sandwich theorem with A_i and $A_{i,0}$ arbitrary.) This comparison suggests that in carrying out the quantization process it will be useful to think of the field variables γ_{ij} as being analogous to the field variables A_i of electromagnetism.

III. INITIAL VALUE EQUATIONS

Einstein's gravitational field equations may be written

$$(-g)^{1/2}[R^{\mu\nu} - \tfrac{1}{2}g^{\mu\nu}R] = 8\pi\tilde{T}^{\mu\nu}, \tag{3.1a}$$

$$\tilde{T}^{\mu\nu}{}_{;\nu} = 0, \tag{3.1b}$$

where $\tilde{T}^{\mu\nu}$ is the energy–momentum tensor density. Equations (3.1b) are a consequence of Eqs. (3.1a). Equations (3.1) may be rewritten in the form

$$R_{ij} = 8\pi(-g)^{-1/2}[\tilde{T}_{ij} - \tfrac{1}{2}g_{ij}\tilde{T}], \tag{3.2a}$$

$$[(-g)^{1/2}(R^0{}_\lambda - \tfrac{1}{2}\delta^0{}_\lambda R) - 8\pi\tilde{T}^0{}_\lambda]_{x^0=\text{const}} = 0, \tag{3.2b}$$

$$\tilde{T}^{\mu\nu}{}_{;\nu} = 0, \quad \text{where} \quad i,j = 1,2,3; \quad \mu,\nu = 0,\dots,3, \tag{3.2c}$$

and the signature of $g_{\mu\nu}$ is $- + + +$. The four equations (3.2b), which are entirely devoid of the second time derivatives of the $g_{\mu\nu}$, are referred to as the initial value equations. They constitute a constraint on the permissible values of the gravitational field on a spacelike three–surface. These four equations may be written in the following form[12] which (a) involves only spatial tensors, and (b) possesses general covariance with respect to coordinate transformations within the initial hypersurface $x^0 = \text{const}$.

$$\gamma^{1/2}[N^{-1}(Q^{ij} - \gamma^{ij}Q^m{}_m)]_{|j} = 8\pi N^{-1}(\gamma^{1/2}S^i), \tag{3.3a}$$

$$\gamma^{1/2}[(Q^i{}_i)^2 - Q_j{}^iQ_i{}^j - (N)^2\bar{R}] = 16\pi(N)^2(\gamma^{1/2}T^0{}_0), \tag{3.3b}$$

where

$$2Q_{ij} = \gamma_{ij,0} - N_{j|i} - N_{i|j} \tag{3.4}$$

and

$$S^i = \gamma^{ki}(N)^2T^0{}_k\,. \tag{3.5}$$

Here γ_{ij} is the spatial metric[13] and the $T^0{}_\mu$ are the components of the energy–momentum tensor $T^\nu{}_\mu$. If one writes $g_{\mu\nu}$ for the metric of spacetime, then

$$\gamma_{ij} = g_{ij}, \quad \gamma^{ij}\gamma_{jk} = \delta^i{}_k\,, \tag{3.6a}$$

$$\gamma^{ij} = g^{ij} - g^{i0}g^{j0}(g^{00})^{-1}, \tag{3.6b}$$

$$N_i = g_{0i}, \quad N = (-g^{00})^{-1/2}, \quad (-g)^{1/2} = N\gamma^{1/2}, \tag{3.6c}$$

where γ denotes the determinant of the spatial metric γ_{ij}. Note that covariant differentiation in Eqs. (3.3) and (3.4) is with respect to γ_{ij}. Raising and lowering of indices is done using γ_{ij}. Also note that both sides of Eqs. (3.3) are spatial densities, and can easily be converted to spacetime tensor densities through multiplication with an appropriate power of N. In the present notation, the spatial Ricci tensor formed from the γ_{ij} is denoted by $\bar{R}^k{}_m$ and the spatial Ricci scalar by $\bar{R}$. The spacetime Ricci tensor is defined by

$$R_{\mu\nu} = (\Gamma^\alpha_{\mu\nu})_{,\alpha} - (\Gamma^\alpha_{\mu\alpha})_{,\nu} + \Gamma^\alpha_{\mu\nu}\Gamma^\beta_{\alpha\beta} - \Gamma^\alpha_{\mu\beta}\Gamma^\beta_{\nu\alpha}, \tag{3.7}$$

where

$$\Gamma^\alpha_{\mu\nu} = \tfrac{1}{2}g^{\alpha\beta}[g_{\mu\beta,\nu} + g_{\nu\beta,\mu} - g_{\mu\nu,\beta}], \tag{3.8}$$

while the spatial Ricci tensor $\bar{R}_{ij}$ is defined by

$$\bar{R}_{jk} = (\bar{\Gamma}^i_{jk})_{,i} - (\bar{\Gamma}^i_{ji})_{,k} + \bar{\Gamma}^i_{jk}\bar{\Gamma}^m_{im} - \bar{\Gamma}^i_{jm}\bar{\Gamma}^m_{ki}\,, \tag{3.9}$$

where

$$\bar{\Gamma}^i_{jk} = \tfrac{1}{2}\gamma^{im}(\gamma_{jm,k} + \gamma_{km,j} - \gamma_{jk,m}). \tag{3.10}$$

Throughout the present paper, spatial covariant differentiation is denoted by a vertical bar while spacetime covariant differentiation is denoted by a semicolon. Equation (3.9) implies the following familiar identity which will be useful later on:

$$\gamma^{lm}(N_{l|km} - N_{l|mk}) = \bar{R}_{ik}N^i. \tag{3.11}$$

IV. THIN–SANDWICH CONJECTURE

The formulation of the thin–sandwich conjecture proved in the present paper was first proposed[4,14] during the years 1962–4. This conjecture states that given the spatial metric and its time rate of change arbitrarily on an initial–value three–surface, there always exists a solution to the initial value Eqs. (3.3) and (3.4). In Sec. I it was noted that this form of the thin–sandwich conjecture has been discussed earlier by Wheeler[4] and Komar.[5] In addition, it should be noted that modified formulations[15] of the thin–sandwich conjecture have been discussed by Komar and Bergmann, and a greatly modified formulation has been discussed by Bruhat.[16] A detailed mathematical review of the work of Komar and Bergmann on modified forms of the thin-sandwich conjecture will be found in the present author's previous paper,[17] in which a new initial value integrability condition was derived from the first three initial value equations (3.3a). The present paper builds on the groundwork laid in the earlier paper and proves some of the unproven expectations given in the earlier paper. In the present paper, all four initial value equations (3.3) will be treated, not just the first three equations as was done earlier.[17]

The energy-momentum tensor $T^{\mu\nu}$ will here be taken to have the form which corresponds to a nonviscous fluid.

$$T^{\mu\nu} = \rho v^\mu v^\nu + p(g^{\mu\nu} + v^\mu v^\nu), \tag{4.1a}$$

where

$$v_\mu v^\mu = -1, \tag{4.1b}$$

and p and ρ are scalars. Then the manner in which ρ, p, v^μ, and γ_{ij} evolve in time is determined from Eqs. (3.2c), (4.1), and (3.2a). For the equations of evolution of the velocity v_i and the density ρ, see Eqs. (32) and (33) or, alternatively, Eqs. (126) of Tauber and Weinberg, Ref. 13. Note, however, that Tauber and Weinberg take the magnitude of the velocity to have a different sign from that used in the present paper.

One may now turn one's attention to the initial value equations (3.2b), written in the form (3.3), and (3.4). Use Eqs. (3.4) to eliminate the Q_{ij} from Eqs. (3.3). One obtains[18]

Highest Derivative

$$2(\gamma^{33})^{-1}\{N^{[A|j]}{}_{|j} - N^{-1}N_{|j}[N^{(A|j)} - \gamma^{Aj}N^i{}_{|i} - E^{Aj}] + \bar{R}^{Aj}N_j - E^{Aj}{}_{|j} + 8\pi S^A\} = 0, \qquad N^A{}_{,33} \tag{4.2a}$$

$$2(\gamma^{33})^{-1}\{N^{[3|j]}{}_{|j} - N^{-1}N_{|j}[N^{(3|j)} - \gamma^{3j}N^i{}_{|i} - E^{3j}] + \bar{R}^{3j}N_j - E^{3j}{}_{|j} + 8\pi S^3\} = 0, \qquad N^2{}_{,32} \tag{4.2b}$$

$$(2N^A{}_{|A} - \gamma^{AB}\gamma_{AB,0})^{-1}[(N^i{}_{|i} - \tfrac{1}{2}\gamma^{ij}\gamma_{ij,0})^2 - (N_{(i|j)} - \tfrac{1}{2}\gamma_{ij,0})(N^{(i|j)} - \tfrac{1}{2}\gamma^{il}\gamma^{jm}\gamma_{lm,0}) - (\bar{R} + 16\pi T^0{}_0)(N)^2] = 0, \qquad N^3{}_{,3} \tag{4.2c}$$

where use has been made of Eq. (3.11) and where the S^i in Eq. (4.2) are given by Eqs. (3.5); and $A = 1,2$. Also note that

$$N^{[n|j]} \equiv \tfrac{1}{2}(N^{n|j} - N^{j|n}), \tag{4.3a}$$

$$N^{(n|j)} \equiv \tfrac{1}{2}(N^{n|j} + N^{j|n}), \tag{4.3b}$$

$$2E_{nj} = \gamma_{nj,0} - \gamma_{nj}\gamma^{im}\gamma_{im,0}\,. \tag{4.4}$$

One may now proceed to prove the following two theorems.

Thin-Sandwich Theorem Ia: For every set of arbitrarily given real analytic functions γ_{ij}, $\gamma_{ij,0}$, p, ρ and v_i there always exists a corresponding set of real analytic functions N^i and N such that Eqs. (4.2), (3.5), and (4.1) are satisfied on the simply connected spacelike hypersurface $x^0 = 0$. Existence is proved in a small but not infinitesimal open region of this hypersurface, and the given functions are functions of the spatial coordinates x^i. In addition, one requires $\gamma \neq 0$ and $\gamma^{33} \neq 0$.

Thin-Sandwich Theorem Ib: For every set of arbitrarily given real analytic functions γ_{ij}, $\gamma_{ij,0}$, $T^0{}_\mu$ there always exists a corresponding set of real analytic functions N^i and N such that Eqs. (4.2) and (3.5) are satisfied on the simply connected spacelike hypersurface $x^0 = 0$. Existence is proved in a small but not infinitesimal open region of this hypersurface, and the given functions are functions of the spatial coordinates x^i. In addition, one requires $\gamma \neq 0$ and $\gamma^{33} \neq 0$.

The proof proceeds as follows. First, assume that the γ^{ij} satisfy the spatial coordinate condition, $\gamma_{3A} = 0$ $(A = 1,2)$, an assumption which it can be shown implies $\gamma^{3A} = 0$. (Note that this coordinate condition is to hold not just at a single point but throughout the region in which existence is to be proved.) This extremely helpful semigeodesic coordinate condition will be removed later on in the proof.

One can now apply Riquier's existence theorem[6] to prove that Eqs. (4.2) have a solution for arbitrary γ_{ij} and $\gamma_{ij,0}$. The first step will be to justify the choice of the highest derivatives[6] given in Eq. (4.2). As in the author's earlier paper, one tries to think of Eqs. (4.2a) and (4.2b) as defining the N^i. One finds that the two Eqs. (4.2a) are then best thought of as defining the derivatives $N^A{}_{,33}$ and that Eq. (4.2b) is then thought of as defining the derivative $N^2{}_{,32}$. This is necessary since the derivatives $N^3{}_{,33}$ and $N^3{}_{,3A}$ are, as will be shown in Appendix B, absent from Eqs. (4.2a) and (4.2b) when $\gamma^{3A} = 0$.

It is now necessary to make a detailed examination of Eq. (4.2c) so as to determine the manner of occurrence of the derivative $N^3{}_{,3}$. To do this without having to write down an equation that would take up too much space, we refer back to Eq. (3.3b) from which Eq. (4.2c) was derived. Equation (3.3b) can be written

$$(-Q^A{}_A)^{-1}[Q^3{}_3(Q^1{}_1 + Q^2{}_2) + Q^1{}_1Q^2{}_2 - Q^1{}_2Q^2{}_1 - Q^1{}_3Q^3{}_1 - Q^2{}_3Q^3{}_2 - (\tfrac{1}{2}\bar{R} + 8\pi T^0{}_0)(N^2)] = 0, \tag{4.5}$$

where

$$Q^i{}_j = \gamma^{im}Q_{jm}\,,$$

and Q_{jm} is an abbreviation for the righthand side of Eq. (3.4). In Appendix B it is shown that in the coordinate system $\gamma^{A3} = 0$, the only $Q^i{}_j$ which contains the derivative $N^3{}_{,3}$ is $Q^3{}_3$. By virtue of this fact, one can, by substituting Eq. (B11) of Appendix B in Eq. (4.5), conclude that $N^3{}_{,3}$ is effectively present in Eq. (4.5) and that it occurs linearly and with coefficient unity. The same result holds for Eq. (4.2c), which, as has been pointed out, is equivalent to Eq. (4.5).

Now consider the full system (4.2). Since Eqs. (4.2a) do not contain the derivatives $N^3{}_{,33}$ or $N^3{}_{,3A}$, it is possible to think of Eq. (4.2c) as defining the derivative $N^3{}_{,3}$. The fact that $N^3{}_{,3}$ is effectively present in Eq. (4.2c) now takes on the greatest importance for the differential structure of the system. The application of Riquier's existence theorem[6] to the full set of four initial value equations (4.2) now leads to an integrability condition. This integrability condition is the same as the integrability condition that was derived for the first three initial value equations in the author's earlier paper.[17] Adding this integrability condition to the original equations, one obtains the following system.[18]

$$N^{[n|j]}{}_{|j} - N^{-1}N_{|j}[N^{(n|j)} - \gamma^{nj}N^i{}_{|i} - E^{nj}] + \bar{R}^{nj}N_j - E^{nj}{}_{|j} = -8\pi S^n, \tag{4.6a}$$

$$[-\bar{R}^n{}_jN^j]_{|n} + N^{-1}N_{|jn}[N^{(n|j)} - \gamma^{nj}N^i{}_{|i} - E^{nj}] + E^{nj}{}_{|jn} = 8\pi N^{-1}(NS^j)_{|j}, \tag{4.6b}$$

$$[N^i{}_{|i} - \tfrac{1}{2}\gamma^{ij}\gamma_{ij,0}]^2 - [N_{(i|j)} - \tfrac{1}{2}\gamma_{ij,0}][N^{(i|j)} - \tfrac{1}{2}\gamma^{il}\gamma^{jm}\gamma_{lm,0}] - (N)^2\bar{R} = 16\pi(N)^2T^0{}_0, \tag{4.6c}$$

where the Q_{ij} and the E_{ij} are given by Eqs. (3.4) and (4.4) respectively. Equations (4.6) have the same solutions as Eqs. (4.2).

Riquier's existence theorem[6,19] is, like the Cauchy–Kowalewsky existence theorem, based on a power series expansion of the unknown functions appearing in a system of partial differential equations. In order to understand the Riquier existence theorem calculations of the present paper, the study of Appendix B and Sec. I of Pereira, Ref. 18, is recommended. The study of Ritt, Ref. 6, Chap. VIII, is also recommended. Note, however, that many of the aspects of Riquier's theorem discussed there, especially the determination of a complete set of monomials associated with the system (4.2), are trivial in the present case and can be ignored. See Eqs. (4.10) and (4.11) for the ordering relationships that are to be used in Eqs. (4.9) and also in Eqs. (4.2).

In Ref. 17 it was noted that Eqs. (4.6a) and (4.6b) can be replaced by an equivalent system in which the third of Eqs. (4.6a) is replaced by an initial condition on the initial value two-surface $x^3 = c_0$. Carrying out this replacement, Eqs. (4.6) become

$$N^{[A|j]}{}_{|j} - N^{-1}N_{|j}[N^{(A|j)} - \gamma^{Aj}N^i{}_{|i} - E^{Aj}] + \bar{R}^{Aj}N_j - E^{Aj}{}_{|j} + 8\pi S^A = 0, \tag{4.7a}$$

$$\{N^{[3|j]}{}_{|j} - N^{-1}N_{|j}[N^{(3|j)} - \gamma^{3j}N^i{}_{|i} - E^{3j}] + \bar{R}^{3j}N_j - E^{3j}{}_{|j} + 8\pi S^3\}_{x^3=c_0} = 0, \tag{4.7b}$$

$$[-\bar{R}^n{}_jN^j]_{|n} + N^{-1}N_{|jn}[N^{(n|j)} - \gamma^{nj}N^i{}_{|i} - E^{nj}] + E^{nj}{}_{|jn} - 8\pi N^{-1}(NS^j)_{|j} = 0, \tag{4.7c}$$

$$[N^i{}_{|i} - \tfrac{1}{2}\gamma^{ij}\gamma_{ij,0}]^2 - [N_{(i|j)} - \tfrac{1}{2}\gamma_{ij,0}] \times [N^{(i|j)} - \tfrac{1}{2}\gamma^{il}\gamma^{jm}\gamma_{lm,0}] - (N)^2[\bar{R} + 16\pi T^0{}_0] = 0, \tag{4.7d}$$

where $i = 1,2,3$; $A = 1,2$; and where the E_{ij} are given by Eqs. (4.4) and

$$S^i = \gamma^{ki}(N)^2T^0{}_k. \tag{4.8}$$

The equivalence between Eqs. (4.7) and (4.6) is familiar in the case where the surface $x^3 = c_0$ is noncompact. It should be noted, however, that if, instead, all the surfaces $x^3 = c$, $c > 0$ are *closed* (i.e., compact and without boundary), then the equivalence between Eqs. (4.7) and (4.6) still holds for all values of x^3, both inside and outside the surface $x^3 = c_0$. This equivalence also holds globally if the three-surface $x^0 = 0$ is itself closed. (This equivalence is, at least in the analytic case, large scale as well as global.) Of course, if the surface $x^0 = 0$ is closed, then the surface $x^3 = c_0$ must also be closed. One must now give an existence proof for the combined system (4.7). The use of Riquier's methods greatly reduces the amount of analysis required. [For a convenient statement of Riquier's theorem, and for a definition of the term *highest derivative* which appears in Eq. (4.9), see Ref. 6.] The final conclusion of the analysis is that it is useful to solve Eqs. (4.7c) and (4.7d) for the derivatives $N_{,33}$ and $N^3{}_{,3}$. The result is given in Eqs. (4.9) below.

Highest Derivative

$$2(\gamma^{33})^{-1}\{N^{[A|j]}{}_{|j} - N^{-1}N_{|j}[N^{(A|j)} - \gamma^{Aj}N^i{}_{|i} - E^{Aj}] + \bar{R}^{Aj}N_j - E^{Aj}{}_{|j} + 8\pi S^A\} = 0, \qquad N^A{}_{,33} \tag{4.9a}$$

$$\{2(\gamma^{33})^{-1}[N^{[3|j]}{}_{|j} - N^{-1}N_{|j}(N^{(3|j)} - \gamma^{3j}N^i{}_{|i} - E^{3j}) + \bar{R}^{3j}N_j - E^{3j}{}_{|j} + 8\pi S^3]\}_{x^3=c_0} = 0, \qquad N^2{}_{,32} \tag{4.9b}$$

$$-(\gamma^{33}N^A{}_{|A} + E^{33})^{-1}\{N_{|jn}[N^{(n|j)} - \gamma^{nj}N^i{}_{|i} - E^{nj}] - N[\bar{R}^n{}_jN^j]_{|n} + NE^{nj}{}_{|jn} + (2N^A{}_{|A} - \gamma^{AB}\gamma_{AB,0})^{-1}(N_{|A}{}^{|A} + N\bar{R}^3{}_3) \times[(N^i{}_{|i} - \tfrac{1}{2}\gamma^{ij}\gamma_{ij,0})^2 - (N_{(i|j)} - \tfrac{1}{2}\gamma_{ij,0})(N^{(i|j)} - \tfrac{1}{2}\gamma^{il}\gamma^{jm}\gamma_{lm,0}) - (N)^2(\bar{R} + 16\pi T^0{}_0)] - 8\pi(NS^j)_{|j}\} = 0, \qquad N_{,33} \tag{4.9c}$$

$$(2N^A{}_{|A} - \gamma^{AB}\gamma_{AB,0})^{-1}[(N_i{}^{|i} - \tfrac{1}{2}\gamma^{ij}\gamma_{ij,0})^2 - (N_{(i|j)} - \tfrac{1}{2}\gamma_{ij,0})(N^{(i|j)} - \tfrac{1}{2}\gamma^{il}\gamma^{jm}\gamma_{lm,0}) - (\bar{R} + 16\pi T^0{}_0)(N)^2] = 0, \qquad N^3{}_{,3} \tag{4.9d}$$

where, as before, the E^{ij} and S^i are given by Eqs. (4.4) and (4.8), respectively, and one is still asked to assume that $\gamma^{A3} = 0$. Equations (4.9) can be considered as having been solved for their highest derivatives. The term *solve* is used here in a generalized sense. Equations (4.9) have been solved for the derivatives $N^A{}_{,33}$; $N^2{}_{,32}$; $N_{,33}$; and $N^3{}_{,3}$ in the sense that each of these derivatives appears in one and only one of the Eqs. (4.9), and if one of these derivatives appears in an equation, it appears linearly and with coefficient unity.

Next apply Riquier's existence theorem to Eqs. (4.9). Because of the nontrivial differential and algebraic complexity of these equations, it is desirable in the present instance to write down the Riquier ordering relationships explicitly. Choose

$$N^3 > N^2 > N^1, \tag{4.10a}$$

$$N_{,3} > N_{,2} > N_{,1}\ , \tag{4.10b}$$

$$N^i{}_{,3} > N^i{}_{,2} > N^i{}_{,1}\ , \tag{4.10c}$$

where the comma denotes partial differentiation. The requirement that the highest derivative in each of the five equations (4.9) be the derivative shown implies the following four pertinent ordering relationships:

from (4.9a) and (4.9b)
$$\begin{cases} N^1{}_{,3} > N^3{}_{,1} > N, & (4.11a)\\ N^2{}_{,3} > N^3{}_{,2} > N, & (4.11b)\end{cases}$$

from (4.9c)

$$N_{,33} > N^2{}_{,3} > N^3{}_{,2}, \tag{4.11c}$$

from (4.9d)

$$N^3_{,3} > N^2{}_{,3} > N^3{}_{,2} > N. \tag{4.11d}$$

All the above ordering relationships can be realized by assigning the following marks or cotes[19] to the independent variables x^i and the dependent variables N, N^i.

variables	x^3	x^2	x^1	N	N^3	N^2	N^1
cotes	(3,0)	(2,0)	(1,0)	(1,3)	(0,3)	(0,2)	(0,1)

(4.11e)

Since Eq. (4.9b) is just an initial condition on a two-surface, one can now conclude[20] that Eqs. (4.9) have no integrability conditions and that they possess a unique real analytic solution in a noncompact simply connected noninfinitesimal region of the three-surface for every choice of the 14 arbitrary real analytic functions of three variables

$$\gamma_{AB},\quad \gamma_{33},\quad \gamma_{ij,0},\quad T^0{}_\mu\ , \tag{4.12}$$

and the six arbitrary real analytic functions of two variables

$$(N^i)_{x^3=c_0},\quad (N^1{}_{,3})_{x^3=c_0},\quad (N)_{x^3=c_0},\quad (N_{,3})_{x^3=c_0}, \tag{4.13}$$

where the two-surface[21] $x^3 = c_0$ is taken to be noncompact and simply connected, and the single arbitrary real analytic function of one variable

$$(N^2{}_{,3})_{x^3=c_0,\ x^2=c_1}\ , \tag{4.14}$$

where the line $x^3 = c_0$, $x^2 = c_1$ is taken to be homeomorphic to R^1 and provided only that (roughly speaking) the denominators of the functions appearing in Eqs. (4.9) are nonzero on the $x^3 = c_0$ surface. In addition, it is assumed that

$$\gamma \neq 0,\quad \gamma^{33} \neq 0,\quad \gamma^{A3} = 0. \tag{4.15}$$

This completes the proof of the Thin–Sandwich Theorem Ib in the special case $\gamma^{A3} = 0$.

To prove Thin–Sandwich Theorem Ia in the special case $\gamma^{A3} = 0$, one must take into account the effects of Eqs. (4.1) on the initial value equations. (Note that Eqs. (3.2a) and (3.2c) are equations of evolution so they need not be considered in the initial value problem.) Equations (4.1a) and (3.5) must be substituted into Eqs. (4.9) to express S^i and $T^0{}_0$ in terms of ρ, p, and v^μ. Since Eq. (4.1b) contains no time derivatives, it fixes the initial determination for the function v_0 on the spacelike initial surface $x^0 = 0$ in terms of the given initial functions v_i, γ_{ij}, N^i, and N on that surface. One must thus rewrite Eq. (4.1b) in the form

$$(v_\mu v^\mu)_{,\alpha} v^\alpha = 0, \tag{4.16a}$$

$$[v_0]_{x^0=0} = \{N^i v_i - [(N)^2\gamma^{ij}v_i v_j + 1]^{1/2}\}_{x^0=0}\ . \tag{4.16b}$$

Equation (4.16a) is an equation of evolution, but Eq. (4.16b) is an initial value equation and therefore implies the Riquier ordering relationships

$$v_0 > N^i,\quad v_0 > N. \tag{4.17}$$

Applying Riquier's existence theorem to the combined system of equations (4.9) and (4.16b), one concludes that this combined system has no integrability conditions and possesses a unique real analytic solution for every choice of the 15 arbitrary real analytic functions of three variables

$$\gamma_{AB},\quad \gamma_{33},\quad \gamma_{ij,0},\quad \rho,\quad p,\quad v_i \tag{4.18}$$

and the six arbitrary real analytic functions of two variables

$$(N^i)_{x^3=c_0},\quad (N^1{}_{,3})_{x^3=c_0},\quad (N)_{x^3=c_0},\quad (N_{,3})_{x^3=c_0}\ , \tag{4.19}$$

where the two-surface[21] $x^3 = c_0$ is taken to be noncompact and simply connected,[22] and the single arbitrary real analytic function of one variable

$$(N^2{}_{,3})_{x^3=c_0,\ x^2=c_1}\ , \tag{4.20}$$

where the line $x^3 = c_0$, $x^2 = c_1$ is taken to be homeomorphic[21] to R^1, and provided only that the denominators of the functions appearing in Eqs. (4.9) and (4.16b) are nonzero on the $x^3 = c_0$ surface. As before, one also assumes that

$$\gamma \neq 0,\quad \gamma^{33} \neq 0, \tag{4.21a}$$

$$\gamma^{A3} = 0. \tag{4.21b}$$

This completes the proof of Thin–Sandwich Theorem Ia in the special case $\gamma^{A3} = 0$.

The final step of the proof of Thin–Sandwich Theorem Ia is to remove assumption (4.21b). Suppose one is given the following system of initial value equations on the three-surface $x^0 = 0$.

$$N^{|n'|j'|}{}_{|j'} - N^{-1}N_{|j'}[N^{(n'|j')} - \gamma^{n'j'}\gamma_{i'm'}N^{(i'|m')} - E^{n'j'}] + \bar{R}^{n'j'}N_{j'} - E^{n'j'}{}_{|j'} + 8\pi S^{n'} = 0, \tag{4.22a}$$

$$N^{-1}N_{|j'n'}[N^{(n'|j')} - \gamma^{n'j'}\gamma_{i'm'}N^{(i'|m')} - E^{n'j'}] - [\bar{R}^{n'}{}_{j'}N^{j'}]_{|n'} + E^{n'j'}{}_{|j'n'} - 8\pi N^{-1}(NS^{j'})_{|j'} = 0, \tag{4.22b}$$

$$[N^{i'}{}_{|i'} - \tfrac{1}{2}\gamma^{i'j'}\gamma_{i'j',0}]^2 - [N_{(i'|j')} - \tfrac{1}{2}\gamma_{i'j',0}][N^{(i'|j')} - \tfrac{1}{2}\gamma^{i'l'}\gamma^{j'm'}\gamma_{l'm',0}] - (N)^2[\bar{R} + 16\pi T^0{}_0] = 0, \tag{4.22c}$$

$$v_0 - N^{i'}v_{i'} + [(N)^2\gamma^{i'j'}v_{i'}v_{j'} + 1]^{1/2} = 0, \tag{4.22d}$$

where the metric components $\gamma^{A'3'}$ in the coordinate system $x^{i'}$ of Eqs. (4.22) need not be zero.

Suppose now that one is also given the 17 arbitrary real analytic functions of three variables

$$\gamma_{i'j'},\quad \gamma_{i'j',0},\quad \rho,\quad p,\quad v_{i'} \tag{4.23}$$

and the six arbitrary real analytic functions of two variables

$$(N^{i'})_{x^{3'}=c_0}, \quad (N^{1'}{}_{,3'})_{x^{3'}=c_0}, \quad (N)_{x^{3'}=c_0}, \quad (N_{,3'})_{x^{3'}=c_0}, \tag{4.24}$$

where the surface $x^{3'} = c_0$ is taken to be noncompact and simply connected and the single arbitrary real analytic function of one variable

$$(N^{2'}{}_{,3'})_{x^{3'}=c_0,\ x^{2'}=c_1} \tag{4.25}$$

where the line $x^{3'} = c_0, x^{2'} = c_1$ is taken to be homeomorphic to R^1, and provided only that the denominators of the functions appearing in Eqs. (4.22) are nonzero on the initial value two-surface $x^{3'} = 0$. Also note that it is assumed, in addition, that the positive definite spatial metric $\gamma_{i'j'}$ satisfies the relations

$$\gamma' \neq 0, \tag{4.26a}$$

$$\gamma^{3'3'} \neq 0. \tag{4.26b}$$

Then, as shown in Appendix A, there will exist a uniquely defined nonsingular analytic coordinate transformation to a different coordinate system x^i in which $\gamma^{43} = 0$. Furthermore, this coordinate transformation will transform Eqs. (4.22) into Eqs. (4.9) and (4.16b), including the restrictions (4.15). In addition, this coordinate transformation will transform the functions (4.23) into analytic functions of the form (4.18). Also, it can be shown that giving the initial conditions (4.24) and (4.25) completely determines the functions of two variables and one variable given in Eqs. (4.19) and (4.20), respectively. Proceeding as before, one concludes that the functions

$$N^i, \quad N(x^i), \quad v_0(x^i) \tag{4.27}$$

defined by the system of Eqs. (4.9) and (4.16b) exist and are analytic. But since one has already demonstrated the existence of the uniquely defined nonsingular real analytic coordinate transformation of Appendix A, that coordinate transformation can be inverted and the inverse transformation used to obtain the analytic functions

$$N^{i'}, \quad N(x^{i'}), \quad v_0(x^{i'}) \tag{4.28}$$

from the functions (4.27). This proves the existence of the functions (4.28) defined by Eqs. (4.22) with the given arbitrary functions (4.23), (4.24), and (4.25), and thus *completes the proof of Thin–Sandwich Theorem* Ia. Note that the proof is also valid in the vacuum case $\rho = p = 0$, and that it is assumed that Eqs. (4.1a) and (3.5) have been substituted into Eqs. (4.22) to express $S^{i'}$ and $T^0{}_0$ in terms of $\rho, p, v^{i'}, v^0 = v^{0'}$, $\gamma_{i'j'}, N^{i'}$, and N. (The case $p = 0, \rho \neq 0$ is not discussed here.)

The same argument used to remove the requirement $\gamma^{43} = 0$ in the proof of Thin–Sandwich Theorem Ia can also be used to remove the requirement $\gamma^{43} = 0$ in the proof of existence for the system of Eqs. (4.9). As before, the requirements (4.26) are assumed. *This completes the proof of Thin–Sandwich Theorem* Ib. Note that the proof is also valid in the vacuum case $T^0{}_\mu = 0$.

The present proofs demonstrate local uniqueness to the initial value problem once the initial conditions of the form (4.24) and (4.25) have been chosen. Also, it is to be emphasized that no coordinate conditions on the metric appear in the final statement of the theorems proved here. Also note that the quantities N^i and N which appear here need not be small. Indeed, it is clear from Eq. (3.6c) that N will usually be close to one.

Regarding global existence, uniqueness, and ellipticity, one may note the following.[23] If a global analytic solution exists then a local analytic solution must also exist. Hence a test for local existence is a necessary but not sufficient test for global existence. A demonstration that there was no local analytic existence for arbitrary γ_{ij} and $\gamma_{ij,0}$ would have destroyed all possibility of global analytic existence for arbitrary γ_{ij} and $\gamma_{ij,0}$.

The present discussion does not demonstrate ellipticity. A careful examination of the existence theorems used here shows that these theorems demonstrate existence whether the equations involved are elliptic or not. (This is to be expected, since Riquier's theorem is an offspring of the Cauchy–Kowalewsky existence theorem.[24]) As one moves across the three-surface, a change in the type of the equations from elliptic to nonelliptic does not destroy existence in the present analytic case. The present results include all real analytic solutions.

One of the main contributions of the present paper toward solving the problem of global existence of solutions to the thin–sandwich equations on a *closed* three-surface (i.e., a three-surface that is compact and without boundary) is the establishment of the fact that the integrability condition (4.6b) can be used to prove nonglobal existence of solutions to the full system of four equations (4.2) and is not limited in its significance to the smaller, incomplete, system of three equations (4.2a) and (4.2b). In the opinion of the author, a careful study of the details of the integrability condition (4.6b) will provide useful guidance in solving the problem of global existence and uniqueness for arbitrary γ_{ij} and $\gamma_{ij,0}$. Equation (4.6b) was derived by local methods, but it holds everywhere and therefore has global significance.

In the opinion of the author, there is in all probability a close relationship between the initial value problem for arbitrary initial functions (4.24) and (4.25) on a noncompact initial two-surface and the boundary value problem[25] for arbitrary choices on a spherical boundary of an appropriately defined set of unknown functions related to the N^i and N. However, since one is here considering a system of partial differential equations which possess integrability conditions, this relationship includes a number of unusual features and is best described in a separate paper. Some of the relationships between the initial value problem and boundary value problems are comparatively obvious, however, and will be noted briefly below.

The present results converge in a region G defined by $c_0 - a < x^3 < c_0 + a$, where the constant a is small but not infinitesimal. Consider a two-sphere Σ of radius $r < b$, with $b < a$, and require that this two-sphere lie within G. Then to every analytic solution to the initial value problem given here, there exists a corresponding analytic solution to the boundary value problem which takes the sphere Σ as the boundary. The present results thus prove the existence of analytic solutions to the boundary value problem (where the bounded region is small but not infinitesimal). However, existence for *arbitrary* boundary values of N^i and N is not proved here; only existence for *some* boundary values is proved. The case of arbitrarily chosen boundary values most be discussed elsewhere. Note that it will not be possible to choose N^i, N, *and* the normal components $\mathbf{n}\cdot\nabla N^i$, $\mathbf{n}\cdot\nabla N$ *arbitrarily* on the sphere Σ and still have a solution everywhere inside Σ. (Here $\mathbf{n}$ is a vector field perpendicular to the surface Σ.)

Also, the present results prove that if an analytic solution on and within Σ is known, then this solution is the *only* analytic solution which has the same values of N^i, N and $\mathbf{n}\cdot\nabla N^i$, $\mathbf{n}\cdot\nabla N$ on Σ. On the other hand, the present results do not prove that the solutions are unique if only N^i and N are given on the sphere Σ.

Now it is known that in the case of a single second order partial differential equation, the solutions to the initial value problem depend continuously on the initial values if the equation is hyperbolic. Also, John[25] has shown that *in the real analytic case*, solutions of a linear second order elliptic equation depend continuously on the initial values. With this in mind, one expects that the *real analytic* solutions whose existence is proved here for the system of nonlinear partial differential equations (4.2) will also depend continuously on the initial values (4.24) and (4.25). However, an actual proof of the fullfillment of this expectation is not given here.

To what extent, on the basis of known results, is it reasonable to hope that the present proof of existence and uniqueness in a noncompact three-dimensional region can be extended so as to prove C^∞ existence on a closed three-surface? To help answer this and other questions, it will be useful to discuss the results of Belasco and Ohanian.[26] Note that the criterion $2\epsilon - R > 0$ used by Belasco and Ohanian ($-[16\pi T^0{}_0 + \bar{R}] > 0$ in the notation of the present paper) is not required to obtain uniqueness in the present discussion. The reason for this is as follows: (a) The problem discussed here is the C^∞ initial value problem within the three-surface, whereas Belasco and Ohanian discuss the Dirchlet problem and do not assume C^∞ boundary values. (b) Consider the thin–sandwich equations discussed by Belasco and Ohanian. The initial value problem within the three-surface corresponding to these equations differs from the corresponding initial value problem discussed here owing to the inclusion of the integrability condition Eq. (4.6b) in the system of equations analyzed here. (The details of the difference are implicit in the discussion of Sec. I of the present paper, since Komar's paper[5] (which is discussed in Sec. I) used the same formulation of the thin-sandwich equations as that used by Belasco and Ohanian.

The requirement $-Q^A{}_A = 2N^A{}_{|A} - \gamma^{AB}\gamma_{AB,0} \neq 0$ that is implicit in Eq. (4.9d) and which is necessary for both existence and uniqueness in the present proof is in agreement with the uniqueness counterexample given in Sec. II of Belasco and Ohanian.

The discussion of the present paper implies that either $T^0{}_i$ or S^i can be specified freely. This is consistent with the first existence counterexample of Sec. III of the paper of Belasco and Ohanian, since existence is proved here only in a noncompact region of the three-surface, whereas Belasco and Ohanian discuss existence throughout a closed simply connected three-surface. The second and third existence counterexamples in Sec. III of Belasco and Ohanian,[26] which at first sight seem to imply that γ_{ij} and $\gamma_{ij,0}$ cannot be chosen arbitrarily on a closed three-surface, are quite misleading. Actually, these counterexamples make the unstated assumption that $N = 1$. Without this special assumption, their conclusions are unjustified.

To summarize then, there are no proven results which imply that γ_{ij} and $\gamma_{ij,0}$ cannot be freely specified on a closed three-surface. However, once γ_{ij} has been chosen there will at least in some circumstances be a global restriction which prevents one from choosing the source terms S^i arbitrarily throughout a simply-connected closed three-surface. [See Eq. (24) of Belasco and Ohanian, Ref. 26.]

Also note that it is assumed here that the spacetime coordinate system is nonsingular. This, of course, implies that the time coordinate x^0 does not lie within the spacelike hypersurface $x^0 = 0$.

Previous authors have obtained a number of global solutions to the initial value equations.[27–28] The local properties of these global solutions are more specialized than the local properties of the solutions whose existence is proved in the present paper because of the local coordinate conditions and local special assumptions[29] which have proven convenient to obtain global results. (Of course, the fact that a given special assumption is *sufficient* to obtain global existence does not imply that this assumption is *necessary* for global existence.) The nonglobal existence theorems of the present paper make no such special assumptions and require no coordinate conditions.

Several authors[14,26] have noted that since the fourth thin–sandwich equation, Eq. (4.2c), is algebraic in N, it can be solved for N. Furthermore, some authors have noted that the fourth equation can be thought of as defining N in terms of the N^i. It should be emphasized that in the present paper, a fifth initial value equation, Eq. (4.6b), is used as an essential part of the existence proof and that this equation contains second derivatives of N. As a result, one is prohibited from considering Eq. (4.2c) to be an equation defining N. The rigorous theoretical framework for this prohibition is Riquier's existence theorem. If one breaks this prohibition, one will find that it is impossible to order the derivatives in the system of five equations (4.6) in such a way as to satisfy the requirements of Riquier's theorem given in Ritt, Ref. 6, Chap. VIII. This prohibition holds not only for the present paper, but also for the author's earlier paper on the thin–sandwich equations.[17,30] (Note that the results proved in this earlier paper allow one to choose the function N arbitrarily. However, this does not imply that the *relationship* between N and the derivatives of the N^i can be chosen arbitrarily.)

The majority of previous discussions of the thin–sandwich conjecture have not included the nonvacuum case. The inclusion of the nonvacuum case $\rho > 0$ in the present proof is partly due to a desire to take into account the fact that *gedanken* experiments which measure the gravitational field cannot be carried out in the absence of matter.[31]

V. ADDITIONAL REMARKS

One motivation for the inclusion of the nonvacuum case in the proof of Thin–Sandwich Theorem Ia of Sec. IV is the desire to allow for possible astrophysical applications. Lichnerowicz[32] has noted that a study of the initial value equations of the gravitational field can be used to improve one's understanding of the dynamics of the general relativistic n-body problem. In the present case, one may note that the arbitrary functions ρ, p, v_i of Theorem Ia, Sec. IV can be chosen so as to describe a very much simplified model of one or more stars in arbitrary relative motion and with arbitrary internal motion at time $x^0 = \text{const.}$, with γ_{ij} and $\gamma_{ij,0}$ also arbitrary. There are a number of examples in which general relativistic effects are believed to play a significant role in stellar structure. These examples include neutron stars,[3,33] supermassive stars,[2] white dwarf stars,[34] and supernova explosions.[3,35]

The form of the energy–momentum tensor used in Eq. (4.1a) of Sec. IV assumes that the matter under consideration is a nonviscous fluid and also neglects any electromagnetic fields which may be present. For a discussion which (a) bears on the viscosity of the fluid present in the interior of neutron stars, (b) describes the role played by the electromagnetic field in the various inner and outer regions of neutron stars, and (c) describes the extent of the solid crust of neutron stars, see Pines, Ref. 1.

Now, in practice, one does not usually choose the density $\rho(x^i)$ and pressure $p(x^i)$ in a stellar model separately as is done in Sec. IV. Instead one may, for example, choose $\rho(x^i)$ and any given equation of state of the form $p = p(\rho)$. It is not difficult to see that Theorem Ia of Sec. IV still implies existence of solutions if, instead of arbitrary p and ρ, one is given arbitrary $\rho(x^i)$ plus an arbitrary equation of state $p = p(\rho)$. For a discussion of an equation of state $p = p(\rho)$ for cold dense matter, see Refs. 36 and 37. For the properties of hot dense matter see Ref. 38.

VI. CONCLUSION

Section IV presents a nonglobal proof of the thin–sandwich conjecture. The results presented here provide the first internally self-consistent proof of the thin–sandwich conjecture which (a) applies for arbitrary choices of the spatial metric and its time derivative; and (b) demonstrates the existence on a spacelike three-surface of solutions which satisfy conditions of continuity known to be sufficient to obtain existence of solutions to Einstein's field equations off the three-surface. Also, it is noted that two different formulations of the thin–sandwich equations are globally equivalent. A comparison of the present results with previous work will be found in Sec. I and at the beginning and end of Sec. IV.

An important feature of the present thin–sandwich existence proof for the four initial value equations (4.2) is that, unlike the existence proof for the first three equations (4.6a) given in Ref. 17, it has in the present proof been necessary to think of the integrability condition (4.6b) as defining the unknown N (rather than defining the unknown N^3 as in Ref. 17).

It should also be noted that as part of the proof the following important features of the initial value equations have been demonstrated: (a) The differential structure of the equations is greatly simplified if one transforms to a semigeodesic coordinate system. The coordinate transformation method used here should also be useful in existence proofs for other systems of generally covariant partial differential equations. (b) In the semigeodesic coordinate system in which $\gamma^{A3} = 0$, the initial value equations (4.9a) and (4.9b) do not contain the derivatives $N^3{}_{,3i}$. (See Appendix B.) (c) In the coordinate system in which $\gamma^{A3} = 0$, the initial value equations (4.9a) do contain the derivatives $N^A{}_{,33}$. (d) In the semigeodesic coordinate system in which $\gamma^{A3} = 0$, the initial value equation (4.9d) is linear in the derivative $N^3{}_{,3}$, and furthermore, this equation contains the quantity $(2Q^A{}_A)$ as a denominator. Additional conclusions are given at the end of Sec. IV.

Riquier's existence theorem and the viewpoint of partial differential algebra play an important role in the present paper. Additional evidence which helps to establish the role of partial differential algebra in the thin–sandwich problem has been obtained in studies carried out by Weinberg.[39]

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APPENDIX A: ON SEMIGEODESIC COORDINATES

One is given 12 arbitrary real analytic functions $\gamma_{i'j'}(x')$ and $\gamma_{i'j',0}(x')$, with $\gamma' \neq 0$ and $\gamma^{3'3'} \neq 0$. It will now be shown that there always exists a real analytic coordinate transformation

$$x^i = f^i(x^{j'}), \quad i = 1,2,3 \tag{A1}$$

to a coordinate system x in which

$$\gamma^{A3} = 0, \quad A = 1,2, \tag{A2}$$

$$\gamma^{33} \neq 0, \quad \gamma \neq 0, \tag{A3}$$

with the γ_{ij} being analytic functions of the x^i. The proof proceeds as follows. Equation (A2) may be written

$$\frac{\partial x^A}{\partial x^{i'}} \frac{\partial x^3}{\partial x^{j'}} \gamma^{i'j'} = 0\,. \tag{A4}$$

Take

$$x^3 = x^{3'}. \tag{A5}$$

Then Eqs. (A4) become

$$\frac{\partial x^A}{\partial x^{3'}} + (\gamma^{3'3'})^{-1} \gamma^{B'3'} \frac{\partial x^A}{\partial x^{B'}} = 0. \tag{A6}$$

Next, apply Cauchy's existence theorem for partial differential equations to Eqs. (A6) and conclude that a unique analytic solution exists to Eqs. (A6) for every analytic choice of the initial conditions

$$[x^A]_{x^{3'} = c_0} = h^A(x^{B'})\,, \tag{A7}$$

where the h^A are arbitrary functions of the $x^{B'}$. It only remains to show that the initial conditions can be chosen so as to make the coordinate transformation (A1) non singular, and unique. To accomplish this, one requires that

$$(x^{A})_{x^{3'}=c_0}=x^{A'} . \quad (A8)$$

This choice (a) guarantees that on the initial surface $x^{3'}=c_0$, the Jacobian of the coordinate transformation (A1) is unity

$$\{|\partial x^{i}/\partial x^{j'}|\}_{x^{3'}=c_0}=1 , \quad (A9)$$

and (b) determines the coordinate transformation (A1) uniquely. Also note that this transformation makes

$$\gamma^{33}=\gamma^{3'3'}\neq 0 . \quad (A10)$$

In addition, it is easy to see [from the analytic nature of the coordinate transformation (A1)] that the nonzero nature of the Jacobian, guaranteed to hold on the initial surface $x^{3'}=c_0$ by virtue of Eq. (A9), must continue to hold for a finite (i.e. noninfinitesimal) distance off the surface. This means that one also has

$$\gamma\neq 0 . \quad (A11)$$

This completes the proof.

The requirement $\gamma^{33}\neq 0$ given at the beginning of this appendix is automatically satisfied by requiring that the spatial metric γ^{ij} be positive definite. For if γ^{ij} is positive definite, then for every real nonzero vector field k_i one has $\gamma^{ij}k_i k_j>0$. Transforming to an arbitrary new nonsingular coordinate system $x^{i'}$, one has $\gamma^{3'3'}=A^{3'}{}_{,i}A^{3'}{}_{,j}\gamma^{ij}>0$, where $A^{3'}{}_{,i}=\partial x^{3'}/\partial x^{i}$ is real and nonzero. Note that one is not allowed to take $A^{3'}{}_{,i}=0$ since this would make the Jacobian $|A^{i'}{}_{,j}|$ of the transformation zero. One concludes that γ^{11}, γ^{22}, and γ^{33} are positive in every nonsingular coordinate system even when γ^{ij} is nondiagonal.

APPENDIX B: FURTHER DETAILS OF THE PROOF

As part of the proofs of Sec. IV it is necessary to make a detailed study of Eqs. (4.2a). The two Eqs. (4.2a) may be written, after multiplication by $\gamma^{1/2}$,

$$[\gamma^{1/2}(N^{A|j}-N^{j|A})]_{|j}=[\cdots] , \quad (B1)$$

where the brackets $[\cdots]$ denote an expression which does not contain any second derivatives of the N^i or N and where one has made use of the fact that

$$(\gamma^{1/2})_{|i}=0 . \quad (B2)$$

Equations (B1) may be written

$$\gamma^{1/2}[\gamma^{33}N^{A}{}_{,33}+2\gamma^{3A}N^{A}{}_{,3A}+\gamma^{BD}N^{A}{}_{,BD}-\gamma^{A3}N^{j}{}_{,3j}-\gamma^{AB}N^{j}{}_{,Bj}]=[\cdots] . \quad (B3)$$

The next step is to put $\gamma^{A3}=0$ in Eqs. (B3). The result is that from an examination of Eqs. (B3) one concludes that when $\gamma^{A3}=0$, the two Eqs. (4.2a) do not contain the derivative $N^{3}{}_{,33}$ and, furthermore, the coefficient of $N^{A}{}_{,33}$ in the two Eqs. (4.2a) is γ^{33}. The third equation Eq. (4.2b) may be written, after multiplication by $\gamma^{1/2}$,

$$[\gamma^{1/2}(N^{3|j}-N^{j|3})_{|j}]=[\cdots] . \quad (B4)$$

Equation (B4) may be written

$$\gamma^{1/2}(2\gamma^{3A}N^{3}{}_{,3A}+\gamma^{AB}N^{3}{}_{,AB}-\gamma^{33}N^{A}{}_{,3A}-\gamma^{3A}N^{j}{}_{,Aj})=[\cdots] . \quad (B5)$$

From an examination of Eq. (B5) one concludes that when $\gamma^{A3}=0$, Eq. (4.2b) contains neither $N^{3}{}_{,33}$ nor $N^{3}{}_{,3A}$ and furthermore, the coefficient of $N^{2}{}_{,32}$ in Eq. (4.2b) is $(-\gamma^{33})$. One therefore requires that $\gamma^{33}\neq 0$.

The importance of the demonstration that $N^{3}{}_{,3A}$ is absent from Eq. (B5) when $\gamma^{A3}=0$ should not be overlooked. Without this demonstration, the existence proof would require that one differentiate Eq. (4.9d) with respect to x^{A} so as to obtain two complicated nonlinear equations for the $N^{3}{}_{,3A}$ in terms of the derivatives $N^{2}{}_{,32}$; $N^{1}{}_{,32}$; $N^{i}{}_{,j}$; etc. One would then have to substitute these equations into Eq. (B5) to eliminate $N^{3}{}_{,3A}$. The result would be that the coefficient of $N^{2}{}_{,32}$ in Eq. (B5) would be a complicated nonlinear expression containing the $N^{i}{}_{,j}$ rather than the simple coefficient γ^{33} which appears in Eq. (B5) when $\gamma^{A3}=0$. Since, as shown in Appendix A, one can assert that $\gamma^{33}\neq 0$ by using the simple physical requirement of a positive definite spatial metric, it is clear that the $\gamma^{A3}=0$ method used here greatly facilitates the proof and furthermore, is not incompatible with the goal of physical transparency.

One may now consider Eqs. (3.4) in the form

$$2Q^{i}{}_{j}=\gamma^{il}(\gamma_{lj,0}-N_{j|l}-N_{l|j}) , \quad (B6)$$

$$2Q^{i}{}_{j}=\gamma^{il}\gamma_{lj,0}-\gamma_{jm}\gamma^{il}N^{m}{}_{|l}-N^{i}{}_{|j} . \quad (B7)$$

In the coordinate system in which $\gamma^{A3}=0$ and $\gamma^{33}\neq 0$, the equation $\gamma_{ij}\gamma^{jk}=\delta^{k}{}_{j}$ implies

$$\gamma_{A3}=0,\quad \gamma_{33}\gamma^{33}=1,\quad A=1,2 . \quad (B8)$$

In this coordinate system, one can, by use of Eqs. (B8), obtain the following:

$$2Q^{3}{}_{A}=\gamma^{33}\gamma_{3A,0}-\gamma_{AB}\gamma^{33}N^{B}{}_{|3}-N^{3}{}_{|A} , \quad (B9)$$

$$2Q^{A}{}_{3}=\gamma^{AB}\gamma_{B3,0}-\gamma_{33}\gamma^{AB}N^{3}{}_{|B}-N^{A}{}_{|3} , \quad (B10)$$

$$2Q^{3}{}_{3}=\gamma^{33}\gamma_{33,0}-2N^{3}{}_{|3} . \quad (B11)$$

Equations (B9) and (B10) show that the only one of the $Q^{i}{}_{j}$ containing $N^{3}{}_{,3}$ is $Q^{3}{}_{3}$.

[1]For a discussion of several aspects of the classical formalism used to formulate the gravitational initial value equations used here, see Sec. II of C.W. Misner, Phys. Rev. **186**, 1319 (1969). The form of the energy-momentum tensor used in Eq. (4.1a) of Sec. IV of the present paper assumes that the gravitating fluid under consideration is nonviscous. For a discussion which bears on the viscosity of the fluid of neutron stars, see D. Pines in, *Proc. 12th International Conference on Low Temperature Physics, Kyoto, Japan*, edited by E. Kanda (Keigaku, Tokyo, 1971). For an example of an equation of state of neutron star matter, see E. E. Salpeter, Astrophys. J. **134**, 669 (1961).

[2]Supermassive stars have been discussed by S. Chandresekhar, Astrophys. J. **140**, 417 (1964); and Philip Morrison, Astrophys. J. (Lett.) L **157**, 73 (1969). It has been suggested that supermassive stars may provide a model for quasi-stellar objects. For details on the redshifts exhibited by a number of quasi-stellar objects see E. M. Burbidge, Astrophys. J. (Lett.) L **160**, 33 (1970).

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[4]See S. W. Hawking and G. F. R. Ellis, *The Large-Scale Structure of Space-Time* (Cambridge U.P., London, 1973), Secs. 7.2, 7.4–7.7, especially pp. 230, 248, 251, 235–6; and p. 33. Special attention should be paid to the

argument on p. 230 which has been overlooked in some recent work. For the existence discussion of Wheeler, see J. A. Wheeler in *Conference internationale sur les théories relativistes de la gravitation*, Warsaw et Jablonna, 1962, edited by L. Infeld, (Gauthier–Villars, Paris, 1964), pp. 245 *et seq.*; and, as an important example of related work, see C. B. Morrey, Jr., Pac. J. Math. **2**, 25 (1952), particularly Theorem 5.1.

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[8]R. P. Feynman, Phys. Rev. **76**, 769–89 (1949), specifically pp. 779–80. As general background for this paper one may examine E. A. Uehling, Phys. Rev. **48**, 55 (1935); and as an interesting example of related work, see L. L. Foldy, Phys. Rev. **93**, 880 (1954).

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[15]A. Komar, Phys. Rev. D **4**, 927 (1971); P. G. Bergmann, GRG **2**, 363 (1971).

[16]Y. Bruhat, Paris C. R. Acad. Sci. A **252**, 3411 (1961). This early result of Bruhat uses a special assumption which permanently destroys the spatial covariance of the initial value equations. This lack of spatial covariance distinguishes this early result from later work and also from the results of the present paper. In a future paper the results of Thin–Sandwich Theorems Ia and Ib of Sec. IV will be used to provide information about the local structure of the superspace which can be associated with solutions of the gravitational initial value equations. For a discussion of superspace see B. S. DeWitt, Phys. Rev. **160**, 1113 (1967); and U. Gerlach, Phys. Rev. **177**, 1929 (1969).

[17]C. M. Pereira, J. Math. Phys. **14**, 1498 (1973). An important clarifying comment regarding this paper is given in Ref. 30. The issues underlying the thin–sandwich problem are closely related to the most fundamental aspects of differential geometry. It is interesting to realize that differential geometry also plays a fundamental role in the geometry of colors. See. J. W. Weinberg, Gen. Relativ. Gravit. **7**, 135 (1976).

[18]Equations (4.2a), (4.2b), and (4.6b) were derived by the author in Ref. 17. It has here been necessary to correct for an inconsistency in the choice of the sign convention in the definition of the Ricci tensor [Eqs. (5), (6), and (8) of Ref. 17]. As background for Ref. 17, see C. M. Pereira, J. Math. Phys. **13**, 1542 (1972).

[19]For Riquier's existence theorem and a definition of *marks* or *cotes*, see Ref. 5 and also J. M. Thomas, *Differential Systems*, Am. Math. Soc. Colloq. Publ., Vol. 21 (Am. Math. Soc., 1937), Chap. 2, Sec. 5. Riquier's existence theorem is closely related to the Cartan–Kähler existence theory. For a comparison of the two theories see J. F. Pommaret, Ann. Inst. Henri Poincaré A **17**, 131–158 (1972), specifically pp. 132–134. An account of recent developments in the Cartan–Kähler theory can be found in J. F. Pommaret, *Systems of Partial Differential Equations and Lie Pseudogroups* (Gordon and Breach, New York, 1978), which contains a bibliography.

[20]A certain amount of additional algebraic and differential manipulation has been deleted here. This manipulation is only necessary if one is interested in the detailed properties of the function spaces associated with the allowed initial conditions on the two-surface $x^3 = c_0$.

[21]Also note that if the two-surface $x^3 = c_0$ is compact then there will, in general, be circumstances in which all of the functions in Eqs. (4.13) and (4.14) cannot be chosen independently if a solution is to exist everywhere within the two-surface. If one takes $x^3 = c_0$ to be homeomorphic to S^2 then the line $x^3 = c_0$, $x^2 = c_1$ would be homeomorphic to S^1. A similar comment can be made regarding Eqs. (4.19) and (4.20).

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[23]For useful comments regarding the relationship between global existence and ellipticity for the case of linear systems of equations, see D. C. Spencer, Bull. Am. Math. Soc. **75**, 179–239 (1969), specifically pp. 179–180. These comments help one to place the results of the present paper in better perspective.

[24]See E. Goursat, *A Course in Mathematical Analysis*, Vol. II, Part 2, *Differential Equations* (Dover, New York, 1959), pp. 283–287 for a statement of the Cauchy–Kowalewsky existence theorem.

[25]For an example of a single second order partial differential equation which exhibits a close relationship between the initial value problem and the boundary value problem, see the interesting results of S. Chandrasekhar, Proc. Cambridge. Philos. Soc. **42**, 250 (1946). For useful comments on second order elliptic equations, see F. John, Commun. Pure Appl. Math. **8**, 591 (1955). Of course, one does not have such continuous dependence on initial values for *nonanalytic* solutions to elliptic equations.

[26]A formulation of the thin–sandwich equations similar to that of Komar, Ref. 5, has been used in the discussion of uniqueness and global questions by E. P. Belasco and H. C. Ohanian, J. Math. Phys. **10**, 1503 (1969). The same unstated special assumption $N = 1$, made by Belasco and Ohanian and discussed in the text, was made more recently (and again is unstated) in Secs. 7–9 of the article of D. Christodoulou and M. Francaviglia, in *Isolated Gravitating Systems in General Relativity. Italian Physical Society Course* 47. *Proc. Int. Sch. of Phys. "Enrico Fermi"*, edited by J. Ehlers (North-Holland, New York, 1979). Thus the claim given in Sec. 1 of the article of Christodoulou and Francaviglia that the global form of the thin–sandwich conjecture is false is also unjustified, since the global thin–sandwich conjecture does not assume that $N = 1$.

[27]See Y. Choquet–Bruhat, Gen. Relativ. Gravit. **5**, 49 (1974) (which contains additional references). Also see C. W. Misner, Phys. Rev. **118**, 1110 (1960); and as examples of related work, see Ref. 28 and D. R. Brill, Ref. 14.

[28]M. D. Kruskal, Phys. Rev. **119**, 1743 (1960); C. Fronsdal, Phys. Rev. **116**, 778 (1959); F. J. Belinfante, Phys. Lett. **20**, 25 (1966).

[29]The special assumptions used to obtain global solutions or other global results usually include one or more of the following: $Q^i{}_i = 0$, $N^i = 0$, $\gamma_{ij,0} = 0$. See for example, Y. Choquet–Bruhat, Ref. 27; R. Geroch, Ann. N. Y. Acad. Sci. **224**, 108 (1973); Y. Choquet–Bruhat and J. W. York (preprint entitled *Cauchy Problem*) to be published in, *General Relativity and Gravitation: Einstein Centenary Volume* (A Publication of the International Society on General Relativity and Gravitation), Chap. 4, edited by A. Held. In some cases, these special assumptions are generalized in one way or another. For example, the special assumption $Q^i{}_i\, N^{-1} = \text{const}$ has been used.

[30]For increased clarity, the following insertion should be made in the author's earlier paper on the thin–sandwich conjecture, C.M. Pereira, J.

Math. Phys. **14**, 1498 (1973). At the bottom of column 1 of page 1499 place the following: "If we remove equation (1b) from the system of Eqs. (1) we are led to consider the following simpler but closely related problem." *Restricted Thin-Sandwich Problem* "Show that for every set of the given functions γ_{ij}, $\gamma_{ij,4}$ and N, there always exists a corresponding set of functions N^i such that Eqs. (1a) are satisfied." The contents of this insertion can be inferred from the paper, but a very careful reading of page 1500 of the paper and a careful reading of the abstract on p. 1498 is required. The quantity Q_{ij} used in the above-mentioned paper and introduced in Sec. III of the present paper is related to the extrinsic curvature (also referred to as the second fundamental tensor) K_{ij} and the canonical momentum density π_{ij} by the equation $K_{ij} = -(N)^{-1}Q_{ij} = -\gamma^{-1/2}(\pi_{ij} - \frac{1}{2}\gamma_{ij}\pi)$. For a discussion of the second fundamental form from a modern mathematical viewpoint, see the article by H. F. Goenner (preprint entitled, *Local Isometric Embedding of Riemannian Manifolds and Einstein's Theory of Gravitation*) to be published in *General Relativity and Gravitation: Einstein Centenary Volume*, edited by A. Held (A Publication of the International Society on General Relativity and Gravitation), Vol. I. I thank Professor Goenner for providing me with a copy of his article before publication. As an interesting example of work related to Goenner's article, see Y. Ne'eman, Rev. Mod. Phys. **37**, 227 (1965).

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[32] A Lichnerowicz, J. Math. Pure Appl. **23**, 37 (1944).

[33] For a discussion of rotating neutron stars as the origin of pulsating radio sources, see T. Gold, Nature **226**, 64 (1970), and for related discussions see E. H. Levy, W. K. Rose, Nature **250**, 40 (1974). For further discussion of phenomena in the vicinity of neutron stars, see E. N. Parker, Astrophys. J. **141**, 1463 (1965).

[34] See J. W. Weinberg and G. E. Tauber, "Gravitational Stability of Large Masses", essay awarded First Prize by Gravity Research Foundation 1963. For a discussion of the composition of white dwarfs see E. J. Öpik, Mem. Soc. R. Sci. Liége **14**, Special No. **131** (1954). Also see W. K. Rose and E. H. Scott, Astrophys. J. **204**, 516 (1976).

[35] See W. A. Fowler and F. Hoyle, Ap. J. Suppl. No. 91, **9**, 201 (1964); W. D. Arnett, Can. J. Phys. **44**, 2553 (1966); and, as background, see I. Iben, Ap. J. **140**, 163 (1964).

[36] See E. E. Salpeter, Ref. 1 and, as background, see M. Gell-Mann and K. Brueckner, Phys. Rev. **106**, 364 (1957).

[37] As background for the last paper of Ref. 36, see M. Gell-Mann, Phys. Rev. **106**, 369 (1957); J. Bardeen, Phys. Rev. **50**, 1098 (1936); and E. P. Wigner, Trans. Faraday Soc. **34**, 678 (1938).

[38] See. D. Q. Lamb, J. M. Lattimer, C. J. Pethick, and D. G. Ravenhall, Phys. Rev. Lett. **41**, 1623 (1978); C. F. McKee, Ap. J. **151**, 647 (1968); and for an interesting example of related work, see P. J. E. Peebles, Ap. J. **146**, 542 (1966).

[39] J. W. Weinberg (unpublished).

Conformally flat static space–time in Brans–Dicke theory

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For the conformally flat spherically symmetric static space–time we obtain the most general solution for Brans–Dicke field equations for a vacuum. By coupling the electromagnetic field to Brans–Dicke theory and imposing the condition of asymptotical flatness we obtain the most general solution for the space–time. We also present some other solutions of Brans–Dicke field equations with the conformally flat condition but without any particular symmetry. Finally, we give the transformation for generating solutions of Brans–Dicke field equations with or without electromagnetic field for $\omega = -3/2$ from purely vacuum solutions of Einstein's field equations.

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1. INTRODUCTION

In a recent communication Reddy[1] attempted to give the most general conformally flat form of the spherically symmetric vacuum solution in the Brans–Dicke theory of gravitation. Unfortunately his procedure is not general, although the final result obtained by him was, by chance, quite general. He had chosen a Minkowskian metric multipled by a conformal factor, which is dependent only on the space coordinates, as the most general spherically symmetric static metric satisfying the conformally flat condition. This is not true in gneral, for example, when the conformally flat Schwarzschild interior static solution is written in this special form of the line element the conformal factor appears as a function of new space as well as time coordinates.[2] In this context we make a more general discussion on the solutions of Brans–Dicke theory representing conformally flat space–time.

In Sec. 2 we have written the most general form of a metric in isotropic coordinates which satisfy the conformally flat condition.

In Sec. 3 we have solved for the conformally flat spherically symmetric static metric for Brans–Dicke field equations.

Finally we arrive at the conclusion that it has unique solution, which is identical with that given by Reddy. The parameter ω attains a fixed value, $-3/2$. Eventually we prove in this connection another result that the most general conformally flat spherically symmetric solution of Einstein's equations for the coupled scalar meson field and gravitation is the trivial solution for flat space–time.

In Sec. 4 we have generalized the result of Sec. 1, including the electromagnetic field. We impose here the condition that the metric must be asymptotically flat and may thus represent the exterior of a source of finite dimension. We obtain the most general conformally flat spherically symmetric static solution for the coupled gravitation and electromagnetic field in Brans–Dicke theory. This solution is valid for all values of ω in the range $(\omega + 3/2) > 0$. The case $\omega = -3/2$ corresponds to a solution which is not asymptotically flat.

In Sec. 5 some other special solutions in Brans–Dicke theory with the conformally flat condition are obtained. Here we do not choose any particular symmetry, though for simplicity have chosen a special form of the metric. In a special case we get a solution which is the static form of the solution given previously by Penney.[3] In another case we can recover the spherically symmetric solution discussed in Sec. 1. There are also other possible solutions.

In Sec. 6 it is shown that one can generate solutions in the Brans–Dicke theory of gravitation, either in the presence of electromagnetic field or in its absence, from purely vacuum solutions of Einstein's field equations by a simple conformal transformation where the parameter ω has a fixed value $-3/2$. This transformation relation has a similarity with that of Janis, Robinson, and Winicour.[4] However, the latter does not consider the unique case $\omega = -3/2$, which we have discussed in this paper.

2. CONFORMALLY FLAT METRICS

A conformastat space–time, as given by Synge,[5] is defined by the line element

$$ds^2 = e^{2\sigma}[-V^2dt^2 + (dx^1)^2 + (dx^2)^2 + (dx^3)^2], \quad (2.1)$$

when

$$V = V(x^1,x^2,x^3)$$

and

$$\sigma = \sigma(x^1,x^2,x^3).$$

In order that a four-dimensional space–time be conformally flat[6] all the components of the associated Weyl tensor

$$\begin{aligned} C^{\alpha}{}_{\delta\gamma\beta} &= R^{\alpha}{}_{\delta\gamma\beta} \\ &+ \tfrac{1}{2}[\delta^{\alpha}{}_{\gamma}R_{\delta\beta} - \delta^{\alpha}{}_{\beta}R_{\delta\gamma} + g_{\delta\beta}R^{\alpha}{}_{\gamma} - g_{\delta\gamma}R^{\alpha}{}_{\beta}] \\ &+ (R/6)[\delta^{\alpha}{}_{\beta}g_{\delta\gamma} - \delta^{\alpha}{}_{\gamma}g_{\delta\beta}] \end{aligned} \quad (2.2)$$

must vanish. We know that if this condition is satisfied for

$$ds^2 = -V^2dt^2 + (dx^1)^2 + (dx^2)^2 + (dx^3)^2, \quad (2.3)$$

then (2.1) is consequently conformally flat. Substituting the metric given by (2.3) into (2.2), the components of the Weyl tensor that do not vanish identically are

$$C_{hook} = -\tfrac{1}{2}VV_{,hk} + \tfrac{1}{6}g_{hk}Vg^{ab}V_{,ab} = 0, \quad (2.4)$$

$$\begin{aligned} C_{hijk} &= (1/2V)[g_{hj}V_{,ik} - g_{hk}V_{,ij} + g_{ik}V_{,hj} - g_{ij}V_{,hk}] \\ &+ (g^{ab}V_{,ab}/3V)[g_{hk}g_{ij} - g_{hj}g_{ik}] = 0. \end{aligned} \quad (2.5)$$

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Greek indices range from 0, 1, 2, 3, and Latin indices 1, 2, 3.

Substituting (2.4) into (2.5), we see that the components (2.5) are identically satisfied. Equation (2.4) may be written

$$\tfrac{1}{3}g^{ab}V_{,ab} = V_{,hk}, \quad \text{for } h = k,$$
$$V_{,hk} = 0, \quad \text{for } h \neq k. \tag{2.6}$$

From (2.6) we have

$$V_{,11} = V_{,22} = V_{,33} = a,$$

which gives, after intergration,

$$V = \tfrac{1}{2}a[(x^1)^2 + (x^2)^2 + (x^3)^2] + b_1x^1 + b_2x^2 + b_3x^3 + c, \tag{2.7}$$

where a, b_1, b_2, b_3, and c are constants.

We have concluded that the space–time given by (2.1) is conformally flat when V is given by (2.7) and σ is an arbitrary function of the space coordinates. It is evident that we can write V as

$$V = \tfrac{1}{2}a[(x^1 + \xi^1)^2 + (x^2 + \xi^2)^2 + (x^3 + \xi^3)^2] + b, \tag{2.8}$$

where ξ^1, ξ^2, ξ^3, and b are constants. By a coordinate transformation the quantity inside the square brackets in (2.8) may be interpreted as a radial coordinate. The general static spherically symmetric metric may be written as

$$ds^2 = e^{2\sigma(r)}[-V^2(r)dt^2 + dr^2 + r^2d\Omega^2]. \tag{2.9}$$

Then, by what had been proved above, the general static conformally flat spherically symmetric metric can be written in isotropic coordinates as

$$ds^2 = e^{2\sigma(r)}[-(ar^2 + b)^2dt^2 + dr^2 + r^2d\Omega^2]. \tag{2.10}$$

3. GENERAL STATIC SPHERICALLY SYMMETRIC CONFORMALLY FLAT SOLUTION OF BRANS–DICKE THEORY

The Brans–Dicke equation in vacuum are

$$G_{\alpha\beta} = -(\omega/\psi^2)[\psi_{,\alpha}\psi_{,\beta} - \tfrac{1}{2}g_{\alpha\beta}\psi_{,\gamma}\psi^{,\gamma}] - (1/\psi)\psi_{;\alpha\beta}, \tag{3.1}$$

$$\Box\psi = 0, \tag{3.2}$$

where ψ is the scalar function. Considering the general static spherically symmetric conformally flat line element (2.10) and assuming ψ as a function of r only, the nonvanishing components of (3.1) are

$$3\sigma'^2 + \frac{4\sigma'}{r} + \frac{4a(1 + r\sigma')}{(b + ar^2)} = \frac{\omega}{2}\left(\frac{\psi'}{\psi}\right)^2 + \frac{\psi''}{\psi} - \sigma'\frac{\psi'}{\psi}, \tag{3.3}$$

$$2\sigma'' + \sigma'^2 + \frac{2\sigma'}{r} + \frac{4a(1 + r\sigma')}{b + ar^2} = -\frac{\omega}{2}\left(\frac{\psi'}{\psi}\right)^2 + \sigma'\frac{\psi'}{\psi} + \frac{1}{r}\frac{\psi'}{\psi}, \tag{3.4}$$

$$2\sigma'' + \sigma'^2 + \frac{4\sigma'}{r} = -\frac{\omega}{2}\left(\frac{\psi'}{\psi}\right)^2 + \sigma'\frac{\psi'}{\psi} + \frac{2ar}{b + ar^2}\frac{\psi'}{\psi}, \tag{3.5}$$

and the wave equation (3.2) becomes

$$\psi'' + \psi'\left(2\sigma' + \frac{2}{r} + \frac{2ar}{b + ar^2}\right) = 0. \tag{3.6}$$

The prime indicate differentiation with respect to r.

It is already shown[7] in the literature that if there exists a functional relationship between g_{00} and the scalar field in static vacuum in Brans–Dicke theory, the relation must be in the form

$$\psi = \psi_0(g_{00})^k,$$

where ψ_0 and k are arbitrary constants. In the present case the functional relationship is trivial because of spherical symmetry and so

$$\psi = \psi_0 e^{2k\sigma}(ar^2 + b)^{2k}. \tag{3.7}$$

Differentiating gives

$$\frac{\psi'}{\psi} = 2k\sigma' + \frac{4kar}{ar^2 + b}. \tag{3.8}$$

Subtracting (3.4) from (3.5), we have

$$\frac{\psi'}{\psi} = -2\sigma' - \frac{4ar}{ar^2 - b}. \tag{3.9}$$

From Eqs. (3.8) and (3.9) we can have σ',

$$\sigma'(1 + k) = -2ar\left(\frac{1}{ar^2 - b} + \frac{k}{ar^2 + b}\right), \tag{3.10}$$

and, differentiating (3.10),

$$\sigma''(1 + k) = -2a\left(\frac{1}{ar^2 - b} + \frac{k}{ar^2 + b}\right) + 2ar\left[\frac{2ar}{(ar^2 + b)^2} + \frac{k\,2ar}{(ar^2 + b)^2}\right]. \tag{3.11}$$

From the wave equation (3.6) and (3.9) we have

$$\frac{\psi''}{\psi'} - \frac{\psi'}{\psi} = \frac{2b(3ar^2 + b)}{r(a^2r^4 - b^2)}. \tag{3.12}$$

Differentiating (3.8), we obtain

$$\frac{\psi''}{\psi'} - \frac{\psi'}{\psi} = \frac{2\sigma'' - 4a(ar^2 + b)/(ar^2 - b)^2}{2\sigma' + 4ar/(ar^2 - b)}. \tag{3.13}$$

Combining (3.12) and (3.13) with the help of (3.10) and (3.11), finally we have

$$\Omega = (1 + k)\Omega, \tag{3.14}$$

where

$$\Omega = \frac{8ab(3a^2r^4 + b^2) + 16ab^2r(3ar + b)}{a^2r^4 - b^2}. \tag{3.15}$$

We see that (3.14) is satisfied either if $k = 0$, which implies flat space–time, or if $\Omega = 0$, and this is true only if either $a = 0$ or $b = 0$. When $a = 0$, we have Reddy's solution by a suitable coordinate transformation. When $b = 0$, we have from (3.12)

$$\frac{\psi''}{\psi'} - \frac{\psi'}{\psi} = 0, \tag{3.16}$$

which, after integration, we obtain

$$\psi = \psi_0 e^{cr}, \tag{3.17}$$

where ψ_0 and c are constants. With (3.8) and (3.9) we conclude that $k = -1$, hence $e^{2\sigma} \propto e^{-cr}/r^4$. Introducing our solution (3.17) into (3.3) we conclude that $\omega = -\frac{3}{2}$.

The solution obtained for $b = 0$ is

$$ds^2 = e^{-cr}[-a^2dt^2 + (1/r^4)(dr^2 + r^2d\Omega^2)]. \quad (3.18)$$

By making the coordinate transformation $\bar{t} = at$ and $\bar{r} = 1/r$ we obtain the solution

$$ds^2 = e^{-c/\bar{r}}[-d\bar{t}^2 + d\bar{r}^2 + \bar{r}^2d\Omega^2], \quad (3.19)$$

and

$$\psi = \psi_0 e^{c/\bar{r}}, \quad (3.20)$$

which is again the solution previously obtained by Reddy. One can thus arrive at the theorem that (3.19) is the only spherically symmetric vacuum solution in Brans–Dicke theory, which is conformally flat. This solution is also asymptotically flat.

One may wonder if one can obtain a confomally flat spherically symmetric solution for a coupled gravitational and scalar meson field in Einstein's theory by applying the transformations of Janis, Robinson, and Winicour[4] to our solutions (3.19) and (3.20). Unfortunately, one cannot obtain such solution because in this case $(2\omega + 3) = 0$, and so one cannot apply the said transformation relation for this specific value of ω. However, one can easily write down Einstein's field equations

$$G_{\mu\nu} = k\,[\,\psi_{,\mu}\psi_{,\nu} - \tfrac{1}{2}g_{\mu\nu}\psi^{\alpha}\psi_{,\alpha}], \quad (3.21)$$

for the general conformally flat spherically symmetric metric given by (2.10) and following steps analogous to those shown in this section one can arrive at a purely flat space–time. Thus we can conclude that the most general conformally flat spherically symmetric static solution corresponding the coupled zero mass scalar field in Einstein's theory represents only purely flat space–time.

4. STATIC SPHERICALLY SYMMETRIC CONFORMALLY FLAT SOLUTION OF BRANS–DICKE THEORY COUPLED WITH AN ELECTROSTATIC FIELD

The Brans–Dicke equations in vacuum coupled with an electromagnetic field are

$$G_{\alpha\beta} = -\frac{k}{\phi}E_{\alpha\beta} - \frac{\omega}{\phi^2}[\,\psi_{,\alpha}\psi_{,\beta} - \tfrac{1}{2}g_{\alpha\beta}\psi_{,\gamma}\psi^{\gamma}] - \frac{1}{\phi}\psi_{;\alpha\beta}, \quad (4.1)$$

$$\Box\psi = 0, \quad (4.2)$$

$$F^{\alpha\beta}{}_{;\beta} = 0. \quad (4.3)$$

$E_{\alpha\beta}$, the energy–momentum tensor for the electromagnetic field, is given by

$$E_{\alpha\beta} = \tfrac{1}{4}[\,F_{\alpha\gamma}F_{\beta}{}^{\gamma} - \tfrac{1}{4}g_{\alpha\beta}F_{\gamma\delta}F^{\gamma\delta}], \quad (4.4)$$

where $F_{\alpha\beta}$ is the electromagnetic field tensor

$$F_{\alpha\beta} = A_{\beta,\alpha} - A_{\alpha,\beta}, \quad (4.5)$$

where A_α is the 4-potential. As we want to study static and spherically symmetric solutions, we can choose the components of the 4-potential as being

$$A_\alpha = (\phi,0,0,0), \quad (4.6)$$

where ϕ is a function of r only. The only nonvanishing components of the electromagnetic field tensor (4.5) are now

$$F_{10} = -F_{01} = \phi'(r). \quad (4.7)$$

Now if we seek only those physically meaningful solutions which are asymptotically flat, the line element, (2.10) can be reduced to a much simpler form. Asymptotic flatness requires that when $\bar{r}^2 \equiv e^{2\sigma}r^2$ approaches infinite magnitude, $|g_{00}|$ must approach a constant quantity of finite magnitude. But since

$$g_{00} = -e^{2\sigma}(a^2r^4 + 2abr^2 + b^2),$$

we must have at least a or b equal to zero in order that g_{00} not become indefinitely large at infinitely large distances from the source. If $a = 0$, we get a line element conformal to a Minkowskian form of the metric by a suitable scale transformation of time. If $b = 0$ we can make a coordinate transformation $r' = 1/r$ and $t' = at$ and we again get back the Minkowskian metric multiplied by a conformal factor. Thus we get the line element in this case as

$$ds^2 = e^{2\sigma(r)}[-dt^2 + dr^2 + r^2d\Omega^2],$$

and the nonvanishing components of the field equations (4.1) with the aid of (4.4) and (4.7) become

$$3\sigma'^2 + \frac{4\sigma'}{r} = -\frac{e^{-2\sigma}}{\psi}\phi'^2 + \frac{\omega}{2}\left(\frac{\psi'}{\psi}\right)^2 + \frac{\psi''}{\psi} - \sigma'\frac{\psi'}{\psi}, \quad (4.8)$$

$$2\sigma'' + \sigma'^2 + \frac{2\sigma'}{r} = \frac{e^{-2\sigma}}{\psi}\phi'^2 - \frac{\omega}{2}\left(\frac{\psi'}{\psi}\right)^2 + \frac{1}{r}\frac{\psi'}{\psi} + \sigma'\frac{\psi'}{\psi}, \quad (4.9)$$

$$2\sigma'' + \sigma'^2 + \frac{4\sigma'}{r} = -\frac{e^{-2\sigma}}{\psi}\phi'^2 - \frac{\omega}{2}\left(\frac{\psi'}{\psi}\right)^2 + \sigma'\frac{\psi'}{\psi}; \quad (4.10)$$

and the wave equation (4.2),

$$\psi'' + [2\sigma' + (2/r)]\psi' = 0. \quad (4.11)$$

Maxwell's equations (4.3) reduce to

$$(r^2\phi')' = 0, \quad (4.12)$$

which, after integration, gives

$$\phi = -A/r + B, \quad (4.13)$$

where A and B are constants of integration.

For solving the above set of equations we take the following procedure. After integrating (4.11) once, we obtain

$$\psi' = e^{-2\sigma}(C/r^2), \quad (4.14)$$

where C is a constant of integration. Subtracting Eq. (4.9) from (4.10) and using (4.13) and (4.14), we obtain

$$\psi = -\frac{e^{-2\sigma}}{r^2\sigma'}\left[\frac{A^2}{r} + \frac{C}{2}\right]. \quad (4.15)$$

Differentiating (4.15) with respect to r and using (4.14), we obtain after integration

$$2\sigma' r\left(\frac{A^2}{2} + dr^2\right) = -\left(\frac{C}{2}r + A^2\right), \quad (4.16)$$

where d is a constant of integration. Now substituting (4.13), (4.14), and (4.15) into (4.8), we have

$$2\sigma'\left[\frac{3}{4}\frac{A^4}{r^2}-\frac{C^2}{8}\left(\frac{3}{2}+\omega\right)\right]=-\frac{3A^2}{2r^2}\left(\frac{A^2}{r}+\frac{C}{2}\right). \tag{4.17}$$

Equating (4.16) and (4.17), we obtain

$$3A^2d=-\frac{C^2}{4}\left(\frac{3}{2}+\omega\right). \tag{4.18}$$

If $C=0$, we see from (4.14) that $\psi=$ const. In this case the field equations are reduced to Einstein's electrovacuum equation and it can be shown that the solution is given by[8]

$$e^{2\sigma}=E/r^2, \tag{4.19}$$

where E is a constant.

Assuming $C\neq 0$ and a vanishing electrostatic field, i. e., $A=0$, we have from (4.18) $\omega=-\frac{3}{2}$ and (4.16) gives Reddy's solution.

Assuming $C\neq 0, A\neq 0$, and $\omega=-\frac{3}{2}$ we see from (4.18) that $d=0$ and (4.16) and (4.17) reduce to

$$2\sigma'=-\frac{2}{A^2}\left(\frac{C}{2}+\frac{A^2}{r}\right), \tag{4.20}$$

giving after integration

$$e^{2\sigma}=Fr^{-2}\exp[-(C/A^2)r], \tag{4.21}$$

F being an integration constant.

We see that (4.21) is not an asymptotically flat solution. The general solution, when $A\neq 0, d\neq 0, C\neq 0$, and $\omega\neq-\frac{3}{2}$ may be obtained by integrating equation (4.17). For $\frac{3}{2}+\omega<0$ we obtain an oscillatory solution which we consider unphysical. For $\frac{3}{2}+\omega=h>0$ we obtain

$$e^{2\sigma}=\left(\frac{1-\beta/r}{1+\beta/r}\right)^{c\beta/A^2}\left(1-\frac{\beta^2}{r^2}\right), \tag{4.22}$$

and, applying (4.15), we have

$$\psi=\frac{A^2}{\beta^2}\left(\frac{1+\beta/r}{1-\beta/r}\right)^{C\beta/A^2}, \tag{4.23}$$

where $\beta=(6/h)^{1/2}A^2/C$ and $h=(\omega+3/2)$, which is an asymptotically flat solution.

So we conclude that the only asymptotically flat spherically symmetric solutions of electrovac representing conformally flat space–time in Brans–Dicke theory are the solutions given by (4.22) and (4.23).

5. OTHER SPECIAL SOLUTIONS OF THE BRANS–DICKE THEORY WITH THE CONFORMALLY FLAT CONDITION

We consider the metric in a conformastat form defined by Synge[5] as

$$ds^2=e^{2\sigma}[-V^2dt^2+(dx^1)^2+(dx^2)^2+(dx^3)^2], \tag{5.1a}$$

where

$$V=\tfrac{1}{2}a[(x^1)^2+(x^2)^2+(x^3)^2]+b_1x^1+b_2x^2+b_3x^3+c, \tag{5.1b}$$

with a, b_1, b_2, b_3 and c all constants and $\sigma=\sigma(x^1,x^2,x^3)$. Substituting (5.1a) and (5.1b) into the field equations (3.1) and (3.2) we obtain:

for G_{ij}

$$-g_{ij}\left[\frac{4a}{V}+g^{ab}\left(2\sigma_{,ab}+\sigma_{,a}\sigma_{,b}+2\frac{V_{,a}\sigma_{,b}}{V}\right)\right]$$
$$+2(\sigma_{,ij}-\sigma_{,i}\sigma_{,j})$$
$$=-\frac{\omega}{\psi^2}\psi_{,i}\psi_{,j}-\frac{\psi_{,ij}}{\psi}+\frac{1}{\psi}(\sigma_{,i}\psi_{,j}+\sigma_{,j}\psi_{,i})$$
$$+g_{ij}\left(\frac{\omega}{2}\frac{g^{ab}\psi_{,a}\psi_{,b}}{\psi^2}-\frac{g^{ab}\sigma_{,a}\psi_{,b}}{\psi}\right), \tag{5.2}$$

for G_{44},

$$g^{ab}(2\sigma_{,ab}+\sigma_{,a}\sigma_{,b})$$
$$=g^{ab}\left[-\frac{\omega}{2}\frac{\psi_{,a}\psi_{,b}}{\psi^2}+\frac{1}{\psi}\left(\frac{V_{,a}\psi_{,b}}{V}+\sigma_{,a}\psi_{,b}\right)\right], \tag{5.3}$$

and for the wave equation,

$$g^{ab}\left(\psi_{,ab}+2\sigma_{,a}\psi_{,b}+\frac{b_a\psi_{,b}}{V}\right)=0; \tag{5.4}$$

one further equation that we can have is the trace of (3.1), giving

$$g^{ab}\left(\sigma_{,ab}+\sigma_{,a}\sigma_{,b}+\frac{b_a\sigma_{,b}}{V}\right)=-\frac{\omega}{6}g^{ab}\frac{\psi_{,a}\psi_{,b}}{\psi^2}. \tag{5.5}$$

Equation (5.5) is, however, not an independent equation, but it is sometimes helpful to get exact solutions.

Assuming $g_{11}=g_{22}=g_{33}=e^{2\sigma}$ functionally related to the scalar field ψ and $a=0$ for simplification, the line element and the field equations (5.2)–(5.5) become, respectively,

$$ds^2=e^{2\sigma}\left[-\left(\sum_i b_ix^i+c\right)^2dt^2+(dx^1)^2+(dx^2)^2+(dx^3)^2\right],$$

and for G_{ij},

$$g_{ij}C(\psi)+\psi_{,i}\psi_{,j}A(\psi)+\psi_{,ij}B(\psi)=0, \tag{5.6}$$

for G_{44},

$$g^{ab}\left(\psi_{,a}\psi_{,b}D(\psi)+2\sigma'\psi_{,ab}-\frac{b_a\psi_{,b}}{V\psi}\right)=0, \tag{5.7}$$

for the wave equation,

$$g^{ab}\left(\psi_{,ab}+2\sigma'\psi_{,a}\psi_{,b}+\frac{b_a\psi_{,b}}{V}\right)=0, \tag{5.8}$$

and for the trace

$$g^{ab}\left[\psi_{,a}\psi_{,b}\left(\sigma''+\sigma'^2+\frac{\omega}{6}\frac{1}{\psi^2}\right)+\sigma'\psi_{,ab}+\sigma'\frac{b_a\psi_{,b}}{V}\right]=0, \tag{5.9}$$

where the prime denotes differentiation with respect to ψ and

$$A(\psi)=-2\sigma''+2\sigma'^2-\frac{\omega}{\psi^2}+\frac{2\sigma'}{\psi}, \tag{5.10}$$

$$B(\psi)=-2\sigma'-1/\psi, \tag{5.11}$$

$$C(\psi)=g^{ab}\psi_{,a}\psi_{,b}D(\psi)+2\sigma'g^{ab}\left(\psi_{,ab}+\frac{b_a\psi_{,b}}{V}\right), \tag{5.12}$$

$$D(\psi)=2\sigma''+\sigma'^2+\frac{\omega}{2}\frac{1}{\psi^2}-\frac{\sigma'}{\psi}. \tag{5.13}$$

For $i\neq j$ we have from (5.6)

$$A(\psi)\psi_{,i}\psi_{,j}+B(\psi)\psi_{,ij}=0. \tag{5.14}$$

Now integrating (5.14), provided $A(\psi)\neq 0$, $B(\psi)\neq 0$, we obtain

$$\ln\psi_{,i}=\xi(\psi)+A_i(x^i), \tag{5.15}$$

where ξ is a function of ψ and A_i is a function of x^i alone. Again Eq. (5.15) on further integration yields

$$\int \exp[-\xi(\psi)]d\psi = A_1 + A_2 + A_3, \tag{5.16}$$

where $A_1 = A_1(x^1)$, $A_2 = A_2(x^2)$, and $A_3 = A_3(x^3)$. In other words the scalar field ψ must be a function of u, where $u = A_1 + A_2 + A_3$. With this last consideration Eq. (5.6) may be written for $i = j$,

$$C(\psi) + \psi_{,u} A_{i,ii} B(\psi) + A^2_{i,i}[A(\psi)\psi^2_{,u} + B(\psi)\psi_{,uu}] = 0. \tag{5.17}$$

and, for $i \neq j$,

$$A_{i,i}A_{j,j}[A(\psi)\psi^2_{,u} + B(\psi)\psi_{,uu}] = 0. \tag{5.18}$$

Introducing the trace (5.9) into (5.12), we have

$$C(\psi) = g^{ab}\psi_{,a}\psi_{,b}\left(-\sigma'^2 + \frac{\omega}{6}\frac{1}{\psi^2} - \frac{\sigma'}{\psi}\right). \tag{5.19}$$

For obtaining the solutions of the set of field equations (5.6)–(5.8) we are going to analyse two case, firstly for $C(\psi) = 0$ and secondly for $C(\psi) \neq 0$.

First case, $C(\psi) = 0$: For this case as we have $g^{ab}\psi_{,a}\psi_{,b} \neq 0$, Eq. (5.19) gives

$$\sigma'^2 - \frac{\omega}{6}\frac{1}{\psi^2} + \frac{\sigma'}{\psi} = 0, \tag{5.20}$$

which has the solution

$$e^{2\sigma} = C_1^2 \psi^{-1+f}, \tag{5.21}$$

where C_1 is a constant of integration and

$$f = \pm[1 + 2\omega/3]^{1/2}. \tag{5.22}$$

The solution (5.21) substituted into (5.10) and (5.11) gives

$$A(\psi) = (f/\psi^2)(1-f), \tag{5.23}$$

$$B(\psi) = -f/\psi. \tag{5.24}$$

Here we may have two situations, (a), $f = 0$ which implies $\omega = -\frac{3}{2}$, and (b) the $f \neq 0$.

(a) $C(\psi) = 0$, $1 + 2\omega/3 = 0$. In this case we have from (5.23) and (5.24) $A(\psi) = B(\psi) = 0$, then Eq. (5.14) is identically satisfied and this implies that ψ may not be a function of u. In this case the field equations (5.6)–(5.8) reduce to

$$g^{ab}\left(\psi_{,a}\psi_{,b} - \psi\psi_{ab} - \psi\frac{b_a\psi_{,b}}{V}\right) = 0. \tag{5.25}$$

Any solution of (5.25) together with (5.21) will give the exact vacuum solution in Brans–Dicke theory.

If we assume the practicular situation of spherical symmetry, then σ and ψ are functions of r, $b_a = 0$, and $u = (x^1)^2 + (x^2)^2 + (x^3)^2 = r^2$, then Eq. (5.25) reduces to

$$4r^2(\psi^2_{,u} - \psi\psi_{,uu}) - 6\psi\psi_{,u} = 0. \tag{5.26}$$

The solution of (5.26) is

$$\psi = C_1\exp(C_2/r), \tag{5.27}$$

where C_1 and C_2 are constants of integration. Equation (5.27) is the solution obtained by Reddy.

(b) $C(\psi) = 0$, $1 + 2\omega/3 > 0$. For this case in (5.17) one possibility is the trivial case $A_{i,i} = 0$ and the second is $A_{i,i} \neq 0$ and $A_{i,ii} = 0$ which, by Eq. (5.18), implies

$$A(\psi)\psi^2_{,u} + B(\psi)\psi_{,uu} = 0. \tag{5.28}$$

Integrating $A_{i,ii} = 0$ we have

$$u = A_1 + A_2 + A_3 = g_1x^1 + g_2x^2 + g_3x^3 + g_4, \tag{5.29}$$

where g_1, g_2, g_3, and g_4 are constants of integration. The field equations (5.6) and (5.8) reduce to

$$\psi_{,i}\psi_{,j}(f-1) + \psi\psi_{,ij} = 0, \tag{5.30}$$

$$g^{ab}b_a\psi_{,b} = 0, \tag{5.31}$$

and so the field equation (5.7) is also satisfied in view of (5.22) and (5.30). Considering (5.29), (5.30) and (5.31) become

$$g_ig_j(\psi^2_{,u}(f-1) + \psi\psi_{,uu}) = 0, \tag{5.32}$$

$$g^{ab}b_ag_b = 0. \tag{5.33}$$

At least one of the g_i's must be different from zero and so implies

$$\psi^2_{,u}(f-1) + \psi\psi_{,uu} = 0, \tag{5.34}$$

which has the solution

$$\psi = (C_1u + C_2)^{1/f}, \tag{5.35}$$

where C_1 and C_2 are constants of integration.

In particular when all the b_i's in (5.2) are zero, (5.35) is the solution which can be obtained from the static case of Penney's solution by applying the transformation from Einstein's massless scalar equations to Brans–Dicke theory.[4] Other solutions can also be obtained from (5.21) and (5.35) when the constant quantities b_i's and g_i's are related by the equation (5.33).

Second case, $C(\psi) \neq 0$: If $C(\psi) \neq 0$, by (5.17) it implies that $A_{i,i} \neq 0$. Then Eq. (5.18) becomes

$$A(\psi)\psi^2_{,u} + B(\psi)\psi_{,uu} = 0. \tag{5.36}$$

Introducing (5.36) into (5.17), we have

$$A_{i,ii} = -\frac{C(\psi)}{\psi_{,u}B(\psi)}, \tag{5.37}$$

which in turn means $A_1(x^1)_{,11} = A_2(x^2)_{,22} = A_3(x^3)_{,33}$ and this implies that $A_{i,ii} = k = \text{const} \neq 0$ and on integrating this expression we obtain

$$u = \tfrac{1}{2}k[(x^1)^2 + (x^2)^2 + (x^3)^2] + l_1x^1 + l_2x^2 + l_3x^3 + m, \tag{5.38}$$

where k, l_1, l_2, l_3, and m are constants of integrations.

Now applying (5.38) into the field equations, we obtain, for (5.17) and (5.18), which combined represent (5.6),

$$2k(u+q)D(\psi)\psi^2_{,u} + 2\sigma'[2k(u+q)\psi_{,uu} + 3k\psi_{,u} + p] + kB(\psi)\psi_{,u} = 0, \tag{5.39}$$

$$A(\psi)\psi^2_{,u} + B(\psi)\psi_{,uu} = 0, \tag{5.40}$$

for (5.7),

$$2k(u+q)D(\psi)\psi^2_{,u} + 2\sigma'[2k(u+q)\psi_{,uu} + 3k\psi_{,u}] - p/\psi = 0, \tag{5.41}$$

for (5.8),

$$4k(u+q)\sigma'\psi^2_{,u} + 2k(u+q)\psi_{,uu} + 3k\psi_{,u} + p = 0, \tag{5.42}$$

where

$$p = (\psi_{,u}/V)g^{ij}(kx^i + l_i)b_j,$$

$$q = (l_1^2 + l_2^2 + l_3^2)/2k - m.$$

Subtracting (5.39) from (5.41), we obtain

$$p = k\psi_{,u}. \tag{5.43}$$

Equating p given by (5.43) with p given earlier one arrives at the relation between the constants in the form $C = \Sigma_i l_i b_i / k$. Equating (5.39), (5.40), and (5.42) with (5.43), we obtain

$$\sigma'' - \sigma'^2 + \frac{\omega}{6}\frac{1}{\psi^2} = 0. \tag{5.44}$$

The solutions of equation (5.44) are the following.

If $-2\omega/3 > 1$,

$$e^{2\sigma} = C_2/\phi\,\{\cos[\ln(C_1\phi)]^{-j/2}\}^2, \tag{5.45}$$

where

$$j = (-1 - 2\omega/3)^{1/2},$$

and C_1 and C_2 are constants of integration. This solution we consider unphysical because of its singularities.

If $1 > -2\omega/3$,

$$e^{2\sigma} = [C_1\phi^{\,i} - 1]^{[(1+i)/i - (i-1)/(i - C_1)]}\phi^{(i-1)/C_1}C_2, \tag{5.46}$$

where,

$$i = (1 + 2\omega/3)^{1/2}.$$

For this case the solutions for $\phi(u)$ became rather complicated and not of much physical interest. We just point out that when $\omega = 0$ it implies that ϕ must be constant and then we have flat space–time.

If $1 = -2\omega/3$,

$$e^{2\sigma} = 1/\phi\,[\ln(C_1\phi)]^2 C_2,$$

and the solution for $\phi(u)$ is

$$C_1\phi = \exp(C_3 u).$$

6. CONFORMAL TRANSFORMATION

Assuming the conformal metric

$$g_{\alpha\beta} = (1/\psi)\bar{g}_{\alpha\beta}, \tag{6.1}$$

we can write the Einstein tensor

$$G_{\alpha\beta} = \bar{G}_{\alpha\beta} + \tfrac{3}{2}(1/\psi^2)(\psi_{,a}\psi_{,\beta} - \tfrac{1}{2}g_{\alpha\beta}\psi_{,\gamma}\psi^{,\gamma}) - (1/\psi)[\psi_{;\alpha\beta} - g_{\alpha\beta}\Box\psi], \tag{6.2}$$

where $\bar{G}_{\alpha\beta}$ is given only in terms of $\bar{g}_{\alpha\beta}$. If

$$\Box\psi = 0, \tag{6.3}$$

any vacuum metric $\bar{g}_{\alpha\beta}$ by (6.1) generates a vacuum Brans–Dicke metric $g_{\alpha\beta}$ with $\omega = -\tfrac{3}{2}$.

If $\bar{g}_{\alpha\beta}$ is an electrovacuum metric satisfying

$$\bar{G}_{\alpha\beta} = -8\pi\bar{E}_{\alpha\beta} = -8\pi\left[\bar{F}^{\gamma}{}_{\alpha}\bar{F}_{\gamma\beta} - \frac{1}{4}\bar{g}_{\alpha\beta}\bar{F}_{\gamma\delta}\bar{F}^{\gamma\delta}\right], \tag{6.4}$$

then $g_{\alpha\beta}$ given by (6.1) along with

$$F_{\alpha\beta} = \bar{F}_{\alpha\beta}, \tag{6.5}$$

is a solution of Brans-Dicke–Maxwell fields subjected to the condition (6.3) and $\omega = -\tfrac{3}{2}$.

One particular case is when $\bar{g}_{\alpha\beta}$ is the flat metric, which means that $g_{\alpha\beta}$ is conformaly flat, assuming ψ is only r-dependent, the wave equation (6.3) becomes

$$\frac{\psi''}{\psi'} - \frac{\psi'}{\psi} + \frac{2}{r} = 0, \tag{6.6}$$

which has the solution

$$\psi = \psi_0 e^{(-c/r)}. \tag{6.7}$$

Equation (6.7) is the solution obtained by Reddy.

The above transformation relations are quite analogous to those of Janis, Robinson, and Winicour. However, these cases were not discussed separately by these authors in their paper, although they need separate attention and lead us to some interesting cases.

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Boundary conditions for zero-rest-mass fields in curved space-time: A regularity theorem

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This paper shows that for gravitational radiation from slow-motion, harmonic sources, the formal power series obtained by expanding the $O(\epsilon^5)$ wave-metric functions in inverse powers of r is a valid asymptotic expansion, provided the phase is expressed in terms of a properly strained null coordinate. The theorem proved here is useful for applying outgoing wave conditions in the neighborhood of $\mathscr{I}^+$.

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1. INTRODUCTION

The construction of approximate radiative solutions of the field equations of general relativity requires the imposition of some kind of boundary condition in the wave zone that selects from the totality of all solutions a subset satisfying some physical requirement. Examples of such requirements include 1) no incoming radiation at $\mathscr{I}^-$, 2) purely outgoing waves near $\mathscr{I}^+$, or 3) a condition guaranteeing the causal nature of the field. For waves on *Minkowski* space, the connections among such conditions are well understood: Solutions constructed using a retarded (or "causal") Green's function are outgoing at $\mathscr{I}^+$. Leipold and Walker[1] have further shown that all solutions satisfying a condition to exclude incoming radiation at $\mathscr{I}^-$ are retarded. However, the converse statement is false unless the sources are sufficiently quiet in the infinite past.

In a *curved* space-time, a precise and useable statement of the physical requirements is far from obvious. For *test* fields on asymptotically flat backgrounds, one can in principle construct a retarded Green's function.[2] Bird and Dixon[3] have shown that retarded integrals formed using such Green's functions are finite and that incoming radiation is excluded—provided the sources satisfy certain boundedness conditions in the infinite past. (These conditions resemble those imposed by Leipold and Walker to exclude incoming radiation in the flat-space case.) However, the structure of their integrals near $\mathscr{I}^+$ is unknown.

In the general case, Green's function methods fail because 1) the geometry of space-time is not prescribed but rather is part of the problem; 2) the equations that describe this geometry are nonlinear. Kovacs and Thorne[4] have proposed an iteration scheme in which at each stage one constructs the metric from a retarded integral whose causal Green's function depends on the metric found in the preceeding stage. Unfortunately, even in the case of scalar perturbations of Schwarzschild only the asymptotic behavior of these Green's functions can be expressed in closed form. Furthermore, it is not yet known under what circumstances such an iteration scheme leads to a uniformly valid asymptotic expansion—let alone a convergent one.

Although "retarded solutions" have no precise meaning in fully nonlinear geometrodynamics, one might hope that a notion of causality in general relativity would apply. However, the implications of such a condition for the fields at $\mathscr{I}^-$ are unclear: Imagine a source that is stationary for retarded times $u < u_0$. A seemingly reasonable definition of "causal" solutions would require the field h resulting from such a source to be stationary for all $u < u_0$. However, Geroch[5] has shown that a sourceless field in curved space-time may have zero data at $\mathscr{I}^-$ and yet produce radiation at $\mathscr{I}^+$. Hence, merely specifying "no incoming radiation" may be insufficient to guarantee "causal" solutions, since sourceless radiation might occur at retarded times earlier than u_0.

A further difficulty arises—even when Green's functions are available—with the imposition of conditions at $\mathscr{I}^-$ such as are needed to exclude incoming radiation. All such conditions require a knowledge of the source behavior in the infinite past. However, the source motion cannot be specified *ab initio* but must be determined as part of the problem. Walker and Will[6] have found that a condition for absence of incoming radiation is indeed satisfied by binary systems in a Keplerian orbit subject to perturbations that were calculated by assuming the validity of Burke's[7] radiation reaction potential (expressed in the form given by MTW[8]) into the infinite past. However, this potential is only known to be uniformly valid over 5/2-PN time scales [O (period/ϵ^5)]. The structure of real physical sources such as the binary pulsar PSR 1913 + 16 in the infinite past is uncertain. One would like a result stating that the system's formation has no measurable effect on its current damping rate.

The Walker–Will calculation also ignored large errors (nonuniformities) arising from the divergence of the true space-time characteristics from the flat-space ones actually used. We have found that such nonuniformities can lead to divergent integrals in higher orders. (However, Walker has recently found[9] that use of the correct characteristics does not modify the conclusions of Walker–Will.)

Before trying to find an approximation scheme that will predict the behavior of a system into the infinite past (in order to verify whether or not boundary conditions at $\mathscr{I}^-$ have been satisfied) one can pursue the more modest goal[10] of describing a system to appropriate (i.e., observational) accuracy in some space-time region of interest. In the case of radiation from a system that is small [$O(\epsilon^5)$] compared to a typical wavelength, the method of matched asymptotic ex-

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pansions first used for such a system by Burke[7] appears to have this capability.

To use this method, one needs separate asymptotic expansions in the wave-, near-, and possibly body-zones (the latter if internal gravity is strong[11,12]). In the wave zone, one needs a boundary condition to select out physically acceptable solutions. However, since the complete wave-zone solution includes regions within a few wavelengths of the sources, the wave-zone solutions beyond linearized order will contain both outgoing and incoming parts—the latter due to backscatter off the inhomogeneities of the metric. Only in the limit $r \to \infty$ will the solution contain purely outgoing waves. Thus, our proposed boundary condition (to be made more precise below) is that solutions in the wave zone shall have the *asymptotic* form of outgoing waves.

The problem to be addressed here is that a *formal* series in, e.g., inverse powers of r (with coefficients functions of retardation variable and angle) need not be a valid *asymptotic expansion*. Such an expansion might omit terms of logarithmic order and thus make large errors. Such errors in fact occur when one uses the naive retarded variable $t - r$ out to infinity. This paper shows that, for harmonic, slow-motion sources, the retarded wave-zone solution at $O(\epsilon^5)$ [including $O(\epsilon^8)$ contributions from nonlinear source terms] does have a valid asymptotic expansion of the form

$$e^{i\omega u} \sum r^{-n} C_n(\theta,\phi;\epsilon)\,, \tag{1}$$

provided the retardation variable u is corrected or "strained" to the Schwarzchild form $u = t - r^*$, where $r^* = r + 2m \ln(r - 2m)$.

2. THE THEOREM

The wave-zone fields at $O(\epsilon^8)$, viewed as a perturbation of Minkowski space, have sources arising from nonlinear combinations of the $O(\epsilon^5)$ quadrupole radiation and $O(\epsilon^3)$ static monopole terms. The divergent integrals that these nonlinear sources produce at $O(\epsilon^8)$ in the straightforward expansion can be eliminated by generalizing the form of the wave-zone expansion as follows:

$$g_{\mu\nu} \sim g_{\mu\nu}(x;\epsilon^3) + \epsilon^5 h_{\mu\nu}(x;\epsilon^3)\,. \tag{2}$$

The implicit dependence on ϵ^3 is a way of including the static monopole terms as part of the background. The zeroth-order metric $g_{\mu\nu}$ corresponds to a Schwarzschild solution with mass m proportional to ϵ^3, and the implicit dependence of $h_{\mu\nu}$ on ϵ^3 will be represented by a dependence on m.

Expansion (2) thus reduces the problem to a linearized perturbation of Schwarzschild. Removing a factor $e^{-i\omega t}$, decomposing into $L = 2$ even-parity harmonics, and specializing to Regge–Wheeler gauge gives the familiar[13–15] set of coupled ordinary differential equations. In particular, the metric functions in these equations can all be expressed in terms of a single function $\hat{K}$ (in the notation of Ref. 15) which satisfies the Zerilli equation[16]

$$\frac{d^2\hat{K}}{dr^{*2}} + [\omega^2 - V(r;\epsilon)]\hat{K} = 0\,, \tag{3}$$

$$r^* \equiv r + 2m \ln(r - 2m)\,, \tag{4}$$

where

$$V(r;\epsilon) \equiv (1 - 2m/r)\left[\frac{24r^3 + 24mr^2 + 36m^2r + 18m^3}{r^3(2r + 3m)^2}\right] \tag{5}$$

is an effective potential.

Of course, the Regge–Wheeler gauge is not the usual for radiation problems because it introduces spurious linear (in r) terms near infinity. However, these terms can be removed by transforming to a well-behaved gauge[14] and do not affect our conclusions.

Our theorem can be stated as follows: The Regge–Wheeler metric functions $h = (H, H_1, K)$ have solutions with asymptotic coordinate expansions valid as $r \to \infty$, of the general form

$$h \sim e^{i\omega r^*} \sum c_n r^{-n}\,. \tag{6}$$

The proof applies a theorem due to Erdelyi[17] to Zerilli's Eq. (3): Consider the equation

$$\psi'' + q(r)\psi = 0 \tag{7}$$

and suppose $q(r)$ has an asymptotic expansion in inverse powers of r,

$$q(r) \sim \sum q_n r^{-n}\,. \tag{8}$$

Then 1)

$$\psi \sim e^{\Omega r} \sum c_n r^{-\rho-n}\,, \tag{9}$$

where

$$\Omega^2 + q_0 = 0, \tag{10}$$

$$-2\Omega\rho + q_1 = 0, \tag{11}$$

$$2\Omega n c_n = (\rho + n)(\rho + n - 1)c_{n-1} + \sum_{\nu=2}^{n+1} q_\nu c_{n+1-\nu}, \quad n = 1,2,\ldots \tag{12}$$

is an asymptotic expansion of ψ, and 2) the function

$$z(r) \equiv e^{-\Omega r} r^\rho \psi \sim \sum c_n r^{-n} \tag{13}$$

can be formally differentiated term by term to produce a valid expansion.

To put Zerilli's equation in the form (7), introduce a new dependent variable ψ satisfying

$$\hat{K} = \psi(1 - 2m/r)^{-1/2}\,. \tag{14}$$

The coefficient function $q(r)$ in Eq. (7) then becomes

$$q(r) = (1 - 2m/r)^{-2}[\omega^2 - V + 2mr^{-3} - 3m^2r^{-4}] \tag{15}$$

and the coefficients q_0 and q_1 are

$$q_0 = \omega^2, \tag{16}$$

$$q_1 = 4m\omega^2. \tag{17}$$

Note that our $q(r)$ does have an asymptotic expansion in inverse powers of r. Application of Eqs. (9)–(11) then gives

$$\psi \sim \exp(\pm i\omega[r + 2m \ln(r - 2m) + O(\epsilon^6)]) \sum c_n r^{-n}\,, \tag{18}$$

completing the proof for ψ.

The metric functions H, H_1, and K of Refs. 13–15 are given in terms of K by the following equations:

$$K(r) = g\hat{K} + \hat{R}, \tag{19}$$

$$H_1(r) = \omega(hK + kR), \tag{20}$$

$$H(r) = (2r + 3m)^{-1}[aK + bH_1], \tag{21}$$

where

$$\hat{R}(r) \equiv d\hat{K}/dr^* = (1 - 2m/r)d\hat{K}/dr, \tag{22}$$

$$g(r) \equiv \frac{6r^2 + 6mr + 6m^2}{r^2(2r + 3m)}, \tag{23}$$

$$h(r) \equiv i\frac{-2r^2 + 6mr + 3m^2}{(r - 2m)(2r + 3m)}, \tag{24}$$

$$k(r) \equiv \frac{-ir^2}{r - 2m}, \tag{25}$$

$$a(r) \equiv 2r - \frac{\omega^2 r^4 + m(r - 3m)}{r - 2m}, \tag{26}$$

$$b(r) \equiv i\omega r^2 + \frac{3m}{i\omega r}. \tag{27}$$

These metric functions will have valid expansions of the form (6) provided the derivative $d\psi/dr$ has such an expansion: The various multiplicative factors in Eqs. (19)–(27) have valid expansions in r^{-1}, and in that case the formal substitution of coefficients[17] gives a valid expansion of the desired form. To show that $d\psi/dr$ has an expansion of the form (6), we observe that

$$d\psi/dr = [(\Omega - \rho r^{-1})z(r) + dz/dr]r^{-\rho}e^{\Omega r} \tag{28}$$

and apply the second property of Erdelyi's theorem stated above.

3. CONCLUSIONS

The theorem states that if the correct null coordinate $u = t - r^*$ is used, then the Regge–Wheeler metric functions have valid asymptotic expansion of the form (6) in inverse powers of r. Our result of course applies only to an approximate system of equations, accurate to $O(\epsilon^5)$. At higher orders, it may be necessary to further refine or "strain" the null coordinate u to avoid nonuniformities. Nevertheless, as a statement about approximate fields, our theorem is in some ways more powerful than the usual "peeling theorem", which merely relates the first few coefficients of a formal series to properties of the curvature on $\mathscr{I}^+$. Our result states that the *formal* expansion in inverse powers of r is in fact a valid *asymptotic* expansion, and therefore the errors in the p-term approximation

$$h \sim e^{i\omega r^*} \sum c_n r^{-n} \tag{29}$$

are $o(r^{-p})$. Finally, we note that Erdelyi's theorem implies nothing about the existence of an asymptotic expansion of h near $\mathscr{I}^-$. [Such an expansion of the form (6) with $e^{i\omega r^*}$ replaced by $e^{-i\omega r^*}$ does of course exist for the *advanced* solution of the Zerilli equation.] Furthermore, from the results of Bardeen and Press,[18] one knows that Schwarzschild test fields obeying the regularity assumptions of the Penrose peeling theorem at $\mathscr{I}^+$ do not necessarily obey them at $\mathscr{I}^-$ For these reasons—together with the need to know the sources of the fields in the infinite past—the ideal of "solving the Cauchy problem for prescribed conditions excluding incoming radiation at $\mathscr{I}^-$" does not lend itself to direct calculations using matching techniques. The problem of showing that matching solutions obeying our "causality conditions" also satisfy reasonable physical conditions (such as the exclusion of incoming radiation) must await future work.

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Statistical mechanics of an exactly integrable system

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The equilibrium thermodynamics of the nonlinear Schrödinger model at finite temperature is calculated by means of the quantum inverse method. Working directly in an infinite volume we derive the equation of state and the integral equation which determines the excitation spectrum. This integral equation is found to be closely related to the Gel'fand–Levitan expression for the charge density operator.

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I. INTRODUCTION

Exact solutions to certain completely integrable quantum field theories[1-4] have revealed that the vacuum and other physical states of these theories have a nontrivial structure which is most conveniently described in terms of many-body distributions. For example, in the massive Thirring model[1] the vacuum is a Dirac sea with a nonuniform distribution of filled negative energy modes while the description of excited states entails a "backflow" function which expresses the response of the Dirac sea to the excitation. The technique which has been used to determine these distribution functions, and thus calculate the energy spectrum of the theory, is patterned after the treatment of the δ-function Bose gas by Lieb.[5] First the system is placed in a box of length L and periodic boundary conditions (PBC's) are either imposed on the Bethe ansatz wave functions or obtained from the algebra of scattering data operators in the quantum inverse method.[6-10] For finite L, the PBC's are a complicated set of transcendental equations which restrict the allowed values of rapidity or momentum for the filled modes. Fortunately, in the limit $L\to\infty$, the PBC equations reduce to fairly simple linear integral equations which determine the vacuum distribution and backflow functions. In the relativistic models which have been studied, these integral equations can be solved explicitly by Fourier transformation, leading to exact spectral results.

Although the periodic boundary condition method is quite powerful and leads to exact results, there now appear to be compelling reasons to re-examine the details of the method with a view toward eliminating the use of a finite box entirely. In addition to the obvious aesthetic objection to using a box to compute quantities which ultimately have little to do with the presence or nature of the box, serious practical problems arise in the formulation of the quantum inverse method in a box of finite length. In the infinite volume case $L=\infty$, the algebra of the scattering data operators $a(\xi)$ and $b(\xi)$ is especially simple and leads to elegant properties for the reflection coefficient operator $R(\xi)\sim b(\xi)a^{-1}(\xi)$. [See Eqs. (1.6).] Although the algebra of a and b operators can be derived for finite L, it is more complicated than the $L=\infty$ case (e.g., an extra exchange term appears in the a-b commutator), and simple relations for the R-operators are not obtained. In fact the utility of the R operator seems to be entirely destroyed by the introduction of a finite box. Since the simple properties of the R operator are at the heart of the Gel'fand–Levitan transformation[10] (which is the inverse part of the quantum inverse method), it is apparent that the use of a finite box has serious drawbacks. It would be reassuring and perhaps enlightening if the spectral integral equations which are usually obtained from Bethe ansatz periodic boundary conditions could be derived directly in the infinite volume theory without resorting to a box. In this paper we will show that for the δ-function gas (quantum nonlinear Schrödinger model), such a derivation is not only possible but leads to new insight into the structure of the Gel'fand–Levitan transformation. We find that the Gel'fand–Levitan expression for the charge-density operator $j_0(x)=\phi^*(x)\phi(x)$ is closely related to the spectral integral equation for the finite temperature δ-function gas first derived by Yang and Yang.[11]

The connection between the spectral integral equation and certain almost-forward matrix elements of the charge density operator was pointed out some time ago in the course of a graphical calculation of the partition function [see Ref. 12, Eq. (4.14) *et seq.*]. At the time no means were available for studying these matrix elements directly, and the calculation was carried out by an indirect method using unitarity of the Møller wave operators. Although the calculation in Ref. 12 demonstrated that the spectral integral equation and partition function of the δ-function gas could be obtained without introducing a finite box or periodic boundary conditions, it required a delicate treatment of the $i\epsilon\to 0$ limit in certain singular denominators. The method discussed in this paper utilizes a direct calculation of matrix elements of $j_0(x)$ starting from the Gel'fand–Levitan expression for that operator. It requires no delicacy in the treatment of $i\epsilon$'s (which may in fact be ignored throughout) and exposes a remarkable correspondence between the expansion of $j_0(x)$ in powers of the R and R^* operators and the expansion of the spectral integral equation in powers of its kernel.

The nonlinear Schrödinger model is described by the Hamiltonian

$$H=\int [\partial_x\phi^*\partial_x\phi + c\phi^*\phi^*\phi\phi]\,dx\,, \tag{1.1}$$

where $\phi(x)$ is nonrelativistic boson field with canonical commutation relations

$$[\phi(x),\phi^*(x')]=\delta(x-x')\,. \tag{1.2}$$

The quantum inverse method for this model is implemented through the linear Zakharov–Shabat eigenvalue problem[13]

$$\left(i\frac{\partial}{\partial x}+\tfrac{1}{2}\xi\right)\Psi_1=-\sqrt{c}\,\Psi_2\phi\,, \qquad (1.3a)$$

$$\left(i\frac{\partial}{\partial x}-\tfrac{1}{2}\xi\right)\Psi_2=\sqrt{c}\,\phi^*\Psi_1\,. \qquad (1.3b)$$

The scattering data operators $a(\xi)$ and $b(\xi)$ are defined in terms of the Jost solution $\psi(x,\xi)$ with the properties

$$\begin{pmatrix}1\\0\end{pmatrix}e^{i\xi x/2}\underset{x\to-\infty}{\longleftarrow}\begin{pmatrix}\psi_1(x,\xi)\\ \psi_2(x,\xi)\end{pmatrix}\underset{x\to+\infty}{\longrightarrow}\begin{pmatrix}a(\xi)e^{i\xi x/2}\\ b(\xi)e^{-i\xi x/2}\end{pmatrix} \qquad (1.4)$$

The fundamental operators $R(\xi)$ are given by

$$R(\xi)=(i/\sqrt{c})b(\xi)a^{-1}(\xi) \qquad (1.5)$$

and may be shown to obey the following simple commutation relations:

$$[H,R^*(\xi)]=\xi^2R^*(\xi)\,, \qquad (1.6a)$$

$$R(\xi)R(\xi')=S(\xi'-\xi)R(\xi')R(\xi)\,, \qquad (1.6b)$$

$$R(\xi)R^*(\xi')=S(\xi-\xi')R^*(\xi')R(\xi)+2\pi\delta(\xi-\xi')\,, \qquad (1.6c)$$

where H is the Hamiltonian, and S is the two-body S-matrix

$$S(\xi-\xi')=(\xi-\xi'-ic)/(\xi-\xi'+ic)\,. \qquad (1.7)$$

From these relations we see that the states $|k_1\cdots k_n\rangle$ defined by

$$|k_1\cdots k_n\rangle=R^*(k_1)\cdots R^*(k_n)|0\rangle\,, \qquad (1.8)$$

(where $|0\rangle$ is the vacuum state with $\phi(x)|0\rangle=0$), are eigenstates of the Hamiltonian:

$$H|k_1\cdots k_n\rangle=\left(\sum_{i=1}^{n}k_i^2\right)|k_1\cdots k_n\rangle\,. \qquad (1.9)$$

These states are identical with those obtained previously by means of Bethe's ansatz. The inner product between two such states may be easily obtained from the commutation relations (1.1).

The inverse transformation from the R operators back to the Heisenberg field $\phi(x)$ is accomplished by means of the quantized version of the Gel'fand–Levitan equation. By using the analytic properties in ξ of the Jost solution $\chi(x,\xi)$ with the behavior $\chi(x,\xi)\sim\binom{0}{1}e^{-i\xi x/2}$ as $x\to+\infty$, it was shown in Ref. 10 that the components χ_1 and χ_2 may be expressed as expansions in the operators $R(\xi)$ and $R^*(\xi)$. The asymptotic behavior of χ_1

$$\chi_1(x,\xi)e^{i\xi x/2}\underset{\xi\to\infty}{\longrightarrow}-(\sqrt{c}/\xi)\,\phi(x)+O(1/\xi^2)$$

yields a corresponding series expansion for the field operator $\phi(x)$. Some properties of this expression have been studied in Refs. 10 and 14. In this paper we use a similar series expansion for the charge density operator $j_0(x)=\phi^*(x)\phi(x)$ which comes from the asymptotic behavior of the other Jost solution component,

$$\chi_2(x,\xi)e^{i\xi x/2}\underset{\xi\to\infty}{\longrightarrow}1-\frac{ic}{\xi}\int_x^\infty j_0(x')\,dx'+O\left(\frac{1}{\xi^2}\right). \qquad (1.10)$$

From this and Eq. (40) of Ref. 10, we obtain the result

$$j_0(x)=\sum_{M=0}^{\infty}j_0^{(M)}(x)\,. \qquad (1.11a)$$

where

$$j_0^{(M)}(x)=(-c)^M\int\prod_{i=1}^{M+1}\left\{\frac{dk_i\,dp_i}{(2\pi)^2}\right\}$$

$$\times\frac{(\sum p-\sum k)e^{-i(\sum p-\sum k)x}}{\prod_{i=1}^{M}\{(p_i-k_i-i\epsilon)(p_i-k_{i+1}-i\epsilon)\}(p_{M+1}-k_{M+1}-i\epsilon)}$$

$$\times R^*(p_{M+1})\cdots R^*(p_1)R(k_1)\cdots R(k_{M+1})\,. \qquad (1.11b)$$

In Sec. II the expansion (1.11) will be used to calculate the partition function of a finite temperature gas. The combinatorics of the series is reduced to an integral equation which is just the equation of Yang and Yang. In the $T\to0$ limit this reduces to the results of Lieb. Section III contains some concluding remarks.

II. PARTITION FUNCTION OF δ-FUNCTION GAS

The purpose of this section is to compute the partition function

$$Q(\beta,\mu)=\mathrm{Tr}\,e^{\beta(\mu N-H)}, \qquad (2.1)$$

where $N=\int dx\,\phi^*(x)\phi(x)$ is the number operator, H is the Hamiltonian, β is the inverse temperature, and μ is the chemical potential. Actually we will compute the extensive quantity $\ln Q$, which was shown in Ref. 12 to have the representation

$$\ln Q=\lim_{q\to0}\mathrm{Tr}\,Y(q)e^{\beta(\mu N-H)}, \qquad (2.2)$$

where the operator $Y(q)$ is defined by

$$Y(q)=e^{-iqK}N^{-1}\int_{-\infty}^{\infty}dx\,j_0(x)e^{iNqx}\,. \qquad (2.3)$$

Here $K=\int dx\,x\phi^*(x)\phi(x)$ is the Galilean boost operator with the property $e^{iqK}R^*(k)=R^*(k+q)e^{iqK}$. Note that formally the limit $q\to0$ of $Y(q)$ is the unit operator, and that in diagrammatic language the effect of taking the limit $q\to0$ outside the trace is just to pick out the connected pieces which go to make up $\ln Q$. In the quantum inverse method this representation of $\ln Q$ is very convenient since Eq. (1.11) expresses $j_0(x)$ in terms of the fundamental operators R and R^* which have simple commutation relations with the Hamiltonian. The operator $Y(q)$ commutes with the total momentum operator $P=\tfrac{1}{2}i\int dx\,\phi^*\overleftrightarrow{\partial}_x\phi$, and so when we take the trace the x integration in (2.3) becomes trivial yielding a factor $2\pi\delta(0)$, which we interpret as the spatial extent L. Using the expansion (1.11) for $j_0(x)$ we then find that the pressure $\mathcal{P}=\beta^{-1}\partial\ln Q/\partial L$ may be written as

$$\mathcal{P}=\beta^{-1}\lim_{q\to0}q\,\mathrm{Tr}\,e^{-iqK}Je^{\beta(\mu N-H)}, \qquad (2.4)$$

where the operator J is given by the expansion

$$J=\sum_{M=0}^{\infty}J^{(M)}$$

$$=\sum_{M=0}^{\infty}(-c)^M\int\prod_{i=1}^{M+1}\left\{\frac{dk_i\,dp_i}{(2\pi)^2}\right\}$$

$$\times\frac{R^*(p_{M+1})\cdots R^*(p_1)R(k_1)\cdots R(k_{M+1})}{\prod_{i=1}^{M}\{(p_i-k_i)(p_i-k_{i+1})\}(p_{M+1}-k_{M+1})}\,. \qquad (2.5)$$

That the limit in (2.4) is nonzero is due to the denominators in (2.5), some of which become of order q when we take the trace. In order to compute this trace we need to evaluate the quantity

$$\Lambda^{(M)}(q)=\mathrm{Tr}\, e^{-iqK}R^*(p_{M+1})\cdots R^*(p_1)R(k_1)\cdots R(k_{M+1})e^{\beta(\mu N-H)}, \tag{2.6}$$

which is shown in the Appendix to be given by

$$\Lambda^{(M)}(q)=(-1)^{M+1}\sum_{n_1\cdots n_{M+1}=1}^{\infty}\left[\prod_{i=1}^{M+1}(-1)^{n_i}e^{n_i\beta(\mu-k_i^2)}\times\langle k_{M+1}+n_{M+1}q,\ \ldots,\ k_1+n_1q\,|p_{M+1}\cdots p_1\rangle\{1+O(q)\}\right]. \tag{2.7}$$

The additional terms of order q have no effect as $q\to 0$ and will be omitted in the following.

Let us use this result to evaluate the contribution to the pressure of the first few terms of (2.5). The zeroth term gives

$$\begin{aligned}\mathcal{P}^{(0)}&=-\frac{1}{\beta}\int\frac{dk_1}{2\pi}\sum_{n_1=1}^{\infty}\frac{(-1)^{n_1}}{n_1}e^{n_1\beta(\mu-k_1^2)}\\&=-\frac{1}{\beta}\int\frac{dk_1}{2\pi}\sum_{n_1=1}^{\infty}\frac{(-1)^{n_1}e^{n_1\beta(\mu-k_1^2)}}{n_1}\\&=\frac{1}{\beta}\int\frac{dk_1}{2\pi}\ln(1+e^{\beta(\mu-k_1^2)}),\end{aligned} \tag{2.8}$$

which is just the well-known expression for the pressure of a free *Fermi* gas. This is at first surprising since the explicit powers of c in the expansion (2.5) might indicate that it is a small coupling expansion, so that the zeroth term should give the pressure for a free *Bose* gas. In fact however, we shall find that due to the implicit c-dependence of the operators R, the higher order terms are actually an expansion in the kernel $\Delta(p-q)$ given by

$$\Delta(p-q)=(2c)/[(p-q)^2+c^2], \tag{2.9}$$

which vanishes as $c\to\infty$ but gives $2\pi\delta(p-q)$ as $c\to 0$.

To see this pattern begin, let us consider the next term $\mathcal{J}^{(1)}$ in the series for J. Before taking the trace it is convenient to symmetrize the integrand of $\mathcal{J}^{(1)}$ over k_1 and k_2 and over p_1 and p_2 and then use the commutation relations (1.6) to recover the original ordering of the R's and R^*'s in each term. In this way we obtain

$$\mathcal{J}^{(1)}=\frac{c}{2}\int\frac{dk_1\,dk_2\,dp_1\,dp_2}{(2\pi)^4}\times\frac{R^*(p_2)R^*(p_1)R(k_1)R(k_2)(p_1+p_2-k_1-k_2)(k_1-k_2)(p_2-p_1)}{(p_1-k_1)(p_1-k_2)(p_2-k_1)(p_2-k_2)(k_1-k_2+ic)(p_2-p_1+ic)}. \tag{2.10}$$

After this symmetrization the contributions to the pressure coming from the two terms of the matrix element $\langle k_2+n_2q,\ k_1+n_1q\,|p_2p_1\rangle$ in the trace $\Lambda^{(1)}(q)$ are equal, so that we may replace this matrix element by $2(2\pi)^2\delta(p_1-k_1-n_1q)\delta(p_2-k_2-n_2q)$. We see that possible poles as $q\to 0$ are cancelled by two powers of q in the numerator so that the limit $q\to 0$ is finite and given by

$$\begin{aligned}\mathcal{P}^{(1)}&=\frac{1}{2\beta}\int\frac{dk_1}{2\pi}\frac{dk_2}{2\pi}\frac{2c}{(k_1-k_2)^2+c^2}\sum_{n_1,n_2=1}^{\infty}\frac{n_1+n_2}{n_1n_2}\times\prod_{i=1}^{2}(-1)^{n_i}e^{n_i\beta(\mu-k_i^2)}\\&=\frac{1}{\beta}\int\frac{dk_1}{2\pi}\frac{dk_2}{2\pi}\Delta(k_1-k_2)\sum_{n_1,n_2=1}^{\infty}n_2^{-1}\prod_{i=1}^{2}(-1)^{n_i}e^{n_i\beta(\mu-k_i^2)}\\&=\frac{1}{\beta}\int\frac{dk_1}{2\pi}\frac{dk_2}{2\pi}\Delta(k_1-k_2)\frac{\ln[1+e^{\beta(\mu-k_2^2)}]}{[1+e^{\beta(k_1^2-\mu)}]}\end{aligned} \tag{2.11}$$

Note that by combining $\mathcal{P}^{(0)}$ and $\mathcal{P}^{(1)}$ and expanding in the fugacity $z=e^{\beta\mu}$ [and multiplying by $2\pi\delta(0)\beta$] we recover the well-known result for the second virial coefficient

$$2\pi\delta(0)\int\frac{dk_1}{2\pi}\frac{dk_2}{2\pi}\{\Delta(k_1-k_2)-\pi\delta(k_1-k_2)\}e^{-\beta(k_1^2+k_2^2)}. \tag{2.12}$$

Let us now consider the general Mth term in the series. Although the details are somewhat complicated the essential pattern of the computation is the same; after symmetrizing over $k_1\cdots k_{M+1}$ and over $p_1\cdots p_{M+1}$ the limit $q\to 0$ is seen to be finite and the c-dependence appears only in the form of M kernels $\Delta(k_i-k_j)$. Explicitly we find[15]

$$\begin{aligned}\mathcal{P}^{(M)}=\frac{1}{\beta}\int&\frac{dk_1\cdots dk_{M+1}(-1)^{M+1}}{(2\pi)^{M+1}(M+1)!}\\&\times\sum_{\mathcal{C}_M\in S_M}\sum_{n_i=1}^{\infty}\prod_{i=1}^{M+1}(-1)^{n_i}\frac{e^{n_i\beta(\mu-k_i^2)}}{n_i}n_i^{m_i-1}\\&\times\left(\sum_1^{M+1}n_i\right)\prod_{\{k_i,k_j\}\in\mathcal{C}_M}\Delta(k_i-k_j),\end{aligned} \tag{2.13}$$

where S_M is the set of all collections $\mathcal{C}_M$ of M pairs $\{k_i,k_j\}$ with $i\neq j$ such that each k_i appears in at least one of the pairs $\{k_i,k_j\}$. The integers $m_i\geq 1$ indicate the number of pairs $\{k_i,k_j\}$ which contain k_i. For example, the $M=2$ term may be written explicitly as

$$\mathcal{P}^{(2)}=-\frac{1}{\beta}\int\frac{dk_1\,dk_2\,dk_3}{(2\pi)^3 3!}\sum_{n_1,n_2,n_3=1}^{\infty}\prod_{i=1}^{3}(-1)^{n_i}e^{n_i\beta(\mu-k_i^2)}\times\frac{n_1+n_2+n_3}{n_1n_2n_3}(n_1\Delta_{12}\Delta_{13}+n_2\Delta_{23}\Delta_{21}+n_3\Delta_{31}\Delta_{32}), \tag{2.14}$$

where $\Delta_{ij}\equiv\Delta(k_i-k_j)$. Summing (2.13) over M from zero to infinity and using the symmetry in the k_i and n_i to replace $\sum n_i$ by $(M+1)n_1$ we obtain the desired expression for the pressure

$$\begin{aligned}\mathcal{P}=\frac{1}{\beta}\sum_{M=0}^{\infty}&\frac{(-1)^{M+1}}{M!}\sum_{\mathcal{C}_M\in S_M}\int\frac{dk_1\cdots dk_{M+1}}{(2\pi)^{M+1}}\\&\times\sum_{n_i=1}^{\infty}\prod_{i=1}^{M+1}(-1)^{n_i}e^{n_i\beta(\mu-k_i^2)}n_i^{m_i-2}\\&\times n_1\prod_{\{i,j\}\in\mathcal{C}_M}\Delta(k_i-k_j).\end{aligned} \tag{2.15}$$

We now show that this result may be expressed in terms of a certain nonlinear integral equation. Let us define $\mathcal{P}(k_1,n_1)$ to be the above expression but with the integral $dk_1/2\pi$ and the sum over n_1 suppressed, and let $\mathcal{P}(k_1)$ be $\sum_{n_1=1}^{\infty}\mathcal{P}(k_1,n_1)$. Also we introduce a quantity

$\sigma(k_1)$ which is essentially those terms of $\mathcal{P}(k_1, n_1)$ with $m_1 = 1$ and external factors omitted, i.e.,

$$\sigma(k_1) = \frac{1}{\beta} \sum_{M=1}^{\infty} \frac{(-1)^{M+1}}{M!} \sum_{\mathfrak{C}_M \in S'_M} \int \frac{dk_2 \cdots dk_{M+1}}{(2\pi)^M} \times \sum_{n_2 \cdots n_{M+1}=1}^{\infty} \prod_{i=2}^{M+1} (-1)^{n_i} e^{n_i \beta(\mu - k_i^2)} n_i^{m_i - 2} \times \prod_{\{k_i, k_j\} \in \mathfrak{C}_M} \Delta(k_i - k_j), \qquad (2.16)$$

where S'_M is that subset of S_M whose elements $\mathfrak{C}_M$ have $m_1 = 1$. Then it is a simple combinatorical exercise to verify that these quantities obey the coupled equations

$$\sigma(k_1) = -\frac{1}{\beta} \int \frac{dk_2}{2\pi} \Delta(k_1 - k_2) \mathcal{P}(k_2), \qquad (2.17)$$

and

$$\mathcal{P}(k_1, n_1) = -\frac{1}{\beta} \frac{(-1)^{n_1} e^{n_1 \beta(\mu - k_1^2)}}{n_1} \sum_{m_1=0}^{\infty} \frac{\{-n_1 \beta \sigma(k_1)\}^{m_1}}{m_1!} = -\frac{1}{\beta} \frac{(-1)^{n_1}}{n_1} e^{n_1 \beta(\mu - k_1^2 - \sigma(k_1))}, \qquad (2.18)$$

so that

$$\mathcal{P}(k_1) = \ln[1 + e^{\beta(\mu - k_1^2 - \sigma(k_1))}]. \qquad (2.19)$$

Combining these results we find that the pressure $\mathcal{P}$ is given by

$$\mathcal{P} = \frac{1}{\beta} \int \frac{dk}{2\pi} \ln[1 + e^{\beta(\mu - k^2 - \sigma(k))}], \qquad (2.20)$$

where $\sigma(k)$ obeys the nonlinear integral equation

$$\sigma(k) = -\frac{1}{\beta} \int \frac{dq}{2\pi} \Delta(k - q) \ln[1 + e^{\beta(\mu - q^2 - \sigma(q))}], \qquad (2.21)$$

in agreement with the result first obtained by Yang and Yang using a variational method. The quantity $\epsilon(k)$ used by these authors is related to our $\sigma(k)$ by

$$\epsilon(k) = k^2 - \mu + \sigma(k). \qquad (2.22)$$

We emphasize that our original expansion (2.4) and (2.5) for the pressure, which follows directly from the Gel'fand–Levitan expression for the charge density, corresponds term by term to an expansion of (2.20) in the kernel $\Delta(k_i - k_j)$.

III. DISCUSSION

To summarize, we have found that the structure of the charge density operator $j_0(x)$ when expressed in terms of R-operators by the quantum inverse method, is directly related to the spectral equation which describes the thermodynamics of the system at finite temtemperature and density first derived by Yang and Yang. Using the Gel'fand–Levitan expression (1.11) for $j_0(x)$, the partition function was calculated from (2.2) and (2.3). The expansion (1.11) or (2.5) leads to the expansion (2.15) for the pressure in powers of the kernel Δ. This result was reduced to a single integral (2.20), where $\sigma(k)$ is the solution of the nonlinear integral equation (2.21). The function $\sigma(k)$ is simply related, by Eq. (2.22), to the quantity $\epsilon(k)$ introduced by Yang and Yang.

Some perspective may be added to these results by recalling that the function $\epsilon(k)$ describes not only the pressure but the complete excitation spectrum of the theory. As shown in Ref. 5, the excitations are of two types, particles with energy $\epsilon(k)$ and holes with energy $-\epsilon(k)$. For multiple excitations the energies are additive. In the zero temperature limit these considerations are found to be equivalent to the method of Lieb for computing excitation energies above the ground state. [Note that Eq. (2.21) becomes linear in the limit $\beta \to \infty$. See Ref. 11.] In fact the Yang and Yang method provides a convenient simplification of Lieb's result, with the bare energy of an excited mode and the backflow energy associated with the excitation combined into a single quantity $\epsilon(k)$. A similar simplification may be noted in the calculation of the massive Thirring model spectrum.[1,2] In this case, the Lieb method is used, and the integral equation for the backflow distribution can be solved explicitly. The backflow energy associated with each excited mode combines nicely with the corresponding bare energy to produce a simple result. Again the energy spectrum may be expressed as additive combinations of a single-particle function $\epsilon(\alpha)$, which gives the energy of a mode with rapidity α. From this similarity one suspects that a method like the one described in Sec. II might provide an alternative derivation of the spectral integral equation for the massive Thirring model which does not rely on periodic boundary conditions in a finite box. Such calculations must await an extension of the quantum Gel'fand–Levitan method to this theory.

In recent investigations of exactly integrable relativistic theories,[1-4] calculations have been carried out at zero temperature with emphasis on the construction of eigenstates. The method developed in this paper provides an interesting counterpoint to the usual approach. Here neither periodic boundary conditions nor explicit properties of the eigenstates were used to obtain the integral equation which determines the spectrum. Only the Gel'fand–Levitan formula (1.11) and the algebra of R-operators (1.6) are used. The role of eigenstates is greatly diminished. This may be a useful shift of emphasis for integrable relativistic boson theories (e.g., nonlinear sigma models) where the explicit construction of eigenstates has not been accomplished. It is also worth noting that the use of finite temperature is essential to the results described in this paper. This is apparent from the repeated use of the cyclic property of the Hilbert space trace for the derivation of Eq. (2.7) given in Appendix A. Corresponding expressions at zero temperature would involve vacuum expectation values which have no such cyclic property. Moreover, the series expansion for $\epsilon(k)$ which emerges from the Gel'fand–Levitan approach is not term-by-term finite at zero temperature. Only after summing the series in the form of an integral equation can the $\beta \to \infty$ limit be taken. It may be that, in further investigations of exactly integrable theories, finite temperature calculations can provide a useful tool even for the study of zero-temperature theories.

APPENDIX

In this appendix we show that $\Lambda^{(M)}(q)$, the trace of a product of R's and R^*'s, defined in (2.6) is Eq. (2.7). One way to do this is to use Bethe ansatz states (1.8) to perform the trace at fixed particle number n and then sum over n. Here we will adopt a more formal, but equivalent, method which employs the cyclic property of the trace. First look at the case $M=0$

$$\Lambda^{(0)}(q;p;k)=\mathrm{Tr}e^{-iqK}R^*(p)R(k)e^{\beta(\mu N-H)}. \qquad (A1)$$

Using the cyclic property of the trace and the algebra of the R operators (1.6) we secure the relation

$$\Lambda^{(0)}(q;p,k)=ze^{-\beta k^2}\{2\pi\delta(k+q-p)\,\mathrm{Tr}e^{-iqK}e^{\beta(\mu N-H)} - S(k+q-p)\,\mathrm{Tr}e^{-iqK}R^*(p)R(k+q) \times e^{\beta(\mu N-H)}\}, \qquad (A2)$$

where $z=e^{\beta\mu}$ is the fugacity. Owing to momentum conservation only the zero particle state contributes to the trace in the first term so that

$$\Lambda^{(0)}(q;p,k)=e^{\beta(\mu-k^2)}\{\langle k+q|p\rangle+S(k+q-p)\Lambda^{(0)}(q;p;k+q)\}, \qquad (A3)$$

where we have used $\langle k+q|p\rangle=2\pi\delta(k+q-p)$. Iterating this result we obtain Eq. (2.7) for the case $M=0$

$$\Lambda^{(0)}(q;p;k)=\sum_{n=1}^{\infty}f_n^{(0)}(q,k)\langle k+nq|p\rangle, \qquad (A4)$$

where

$$f_n^{(0)}(q,k)=z^n e^{-\beta k^2}\prod_{l=1}^{n-1}S(lq-nq)e^{-\beta(k+lq)^2} =-(-z)^n e^{-n\beta k^2}+O(q). \qquad (A5)$$

We will prove a similar formula for arbitrary M by induction. Assume $\Lambda^{(M-1)}(q;p_1\cdots p_M,k_1\cdots k_M)$ has the form

$$\Lambda^{(M-1)}(q;\{p_l\},\{k_l\})=\sum_{\{n_l\}=1}^{\infty}f_{\{n_l\}}^{(M-1)}(q,\{k_l\}) \times\langle k_M+n_Mq\cdots k_1+n_1q|p_M\cdots p_1\rangle, \qquad (A6)$$

where

$$f_{\{n_l\}}^{(M-1)}(q,\{k_l\})=(-1)^M\prod_{l=1}^{M}(-z)^{n_l}e^{-n_l\beta k_l^2}+O(q). \qquad (A7)$$

Consider now

$$\Lambda^{(M)}(q,\{p_l\},\{k_l\})\equiv\mathrm{Tr}e^{-iqK}R^*(p_{M+1})\cdots R^*(p_1)R(k_1)\cdots \times R(k_{M+1})e^{\beta(\mu N-H)}. \qquad (A8)$$

Generalizing the previous technique, we cycle $R(k_{M+1})$ to obtain

$$\Lambda^{(M)}(q,\{p_l\},\{k_l\})=\sum+ze^{-\beta k^2_{M+1}}\prod_{j=1}^{M+1}S(k_{M+1}+q-p_j) \times\prod_{l=1}^{M}S^{-1}(k_{M+1}+q-k_l) \times\Lambda^{(M)}(q;\{p_l\};k_1\cdots k_M,k_{M+1}+q), \qquad (A9)$$

where

$$\sum=ze^{-\beta k^2_{M+1}}\sum_{j=1}^{M+1}2\pi\delta(k_{M+1}+q-p_j)\prod_{l=j+1}^{M+1}S(k_{M+1}+q-p_l) \times\Lambda^{(M-1)}(q,p_1\cdots p_{j-1},p_{j+1}\cdots p_{M+1},k_1\cdots k_M)$$
$$=ze^{-\beta k^2_{M+1}}\sum_{\substack{\{n_i\}=1\\ i=1\ldots M}}^{\infty}f_{\{n_i\}}^{(M-1)}(q,\{k_i\}) \times\langle k_{M+1}+n_{M+1}q,k_M+n_Mq\cdots k_1+n_1q|p_{M+1}\cdots p_1\rangle. \qquad (A10)$$

The second equality follows from the inductive hypothesis coupled with the identity

$$\langle q_{M+1}\cdots q_1|p_{M+1}\cdots p_1\rangle=\sum_{j=1}^{M+1}2\pi\delta(q_{M+1}-p_j) \times\prod_{l=j+1}^{M+1}S(q_{M+1}-p_l) \times\langle q_M\cdots q_1|p_{M+1}\cdots p_{j+1},p_{j-1}\cdots p_1\rangle, \qquad (A11)$$

which itself follows from the algebra of the R operators (1.6). Equation (A9) can now be iterated yielding an infinite series for $\Lambda^{(M)}$. If we note that when multiplied by the inner product $\langle k_{M+1}+n_{M+1}q\cdots k_1+n_1q|p_{M+1}\cdots p_1\rangle$ we have the relation

$$\prod_{j=1}^{M}S(k_{M+1}+nq-p_j)\prod_{l=1}^{M}S^{-1}(k_{M+1}+nq-k_l)=-1+O(q), \qquad (A12)$$

then we find

$$\Lambda^{(M)}(q;\{p_l\},\{k_l\})=\sum_{\{n_i\}=1}^{\infty}f_{\{n_i\}}^{(M)}(q,\{k_i\}) \times\langle k_{M+1}+n_{M+1}q\cdots k_1+n_1q|p_{M+1}\cdots p_1\rangle, \qquad (A13)$$

with

$$f_{\{n_i\}}^{(M)}=-(-z)^{n_{M+1}}e^{-n_{M+1}\beta k^2_{M+1}}f_{\{n_i\}}^{(M-1)}+O(q) =(-1)^{M+1}\prod_{l=1}^{M+1}(-z)^{n_l}e^{-n_l\beta k_l^2}+O(q). \qquad (A14)$$

This completes the induction from $M-1$ to M.

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[15]We have not managed to construct a general proof of this result but have verified it for the first four terms of the series. The symmetrization for the $M=2$ and $M=3$ terms were carried out using the algebraic manipulation program MACSYMA.

Note added in proof: We have recently constructed a complete inductive proof of (2.13) which will be given in a subsequent publication.

Amplitudes on von Neumann lattices

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A formula is derived connecting any wave function $\langle k,q|f\rangle$ in the kq-representation with the corresponding amplitudes of the state $|f\rangle$ on von Neumann lattices of states. The formula is used for establishing a possible interpretation for these amplitudes, for obtaining linear relationships between them, and for finding sum rules for the squares of their absolute values, and other related sum rules. It can also be used for establishing completeness criteria for the lattices of states and for defining a modified Hilbert space in which they become strictly complete. Particular attention is given to the coherent state lattice, but the discussion is extended to von Neumann lattices generated from an arbitrary state. Lattices generated from harmonic oscillator states are studied explicitly, and shown incidentally to lead to a wealth of summation expressions for Laguerre polynomials.

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I. INTRODUCTION

Coherent states were first introduced into quantum mechanics by Schrödinger.[1] Later they were shown to form a quantum mechanical representation[2] and be applicable in numerous applications in quantum optics[3] and other fields of quantum physics.[4]

Formally, the coherent states are defined as eigenstates of the annihilation operator

$$\hat{a}=(1/\lambda\sqrt{2})(\hat{x}+(i/\hbar)\lambda^2\hat{p}), \tag{1}$$

where λ is associated with the constants m and ω of a harmonic oscillator, $\lambda^2=\hbar/m\omega$. Unlike $\hat{x}$ or $\hat{p}$, the operator $\hat{a}$ is not Hermitian and its eigenstates, $|\alpha\rangle$, which are the coherent states, are nonorthogonal. Here α is given as follows

$$\alpha=(1/\lambda\sqrt{2})(\bar{x}+(i/\hbar)\lambda^2\bar{p}), \tag{2}$$

where $\bar{x}$ and $\bar{p}$ are the coordinate and momentum expectation values in the state $|\alpha\rangle$. The coherent states $|\alpha\rangle$ form a nonorthogonal and overcomplete set.[2,3] These two features distinguish them from complete orthonormal sets commonly used in quantum mechanics, e.g., the eigenstates of a harmonic oscillator $|N\rangle$. In particular, given a system in the state $|f\rangle$, the scalar product $\langle N|f\rangle$ has a probability interpretation, namely, $|\langle N|f\rangle|^2$ is the probability to find the system in the state $|N\rangle$. Such an interpretation does not hold with respect to coherent states, and the quantity $|\langle\alpha|f\rangle|^2$ can only be given an approximate semiclassical probability interpretation.[5] The latter seems to be a consequence of the overcompleteness and nonorthogonality of the coherent states.

At the very early stages of the development of quantum mechanics von Neumann[6] suggested a physical way of how to choose a subset of coherent states which preserve the property of completeness. Such a subset is obtained by choosing only those states $|\alpha_{mn}\rangle$ which correspond to discrete values α_{mn} of the parameter α in (1)

$$\alpha_{mn}=(1/\lambda\sqrt{2})(na+i(2\pi/a)\lambda^2 m), \tag{3}$$

where m and n are all integers, $m,n=0,\pm1,\pm2$, and a is an arbitrary real constant, The α_{mn} as defined in (3) form a lattice in the phase plane with a unit cell area equal to h, the Planck constant. We shall call this lattice the von Neumann lattice and correspondingly $|\alpha_{mn}\rangle$ will be called a von Neumann lattice of coherent states.

It was later shown[7,8] that the subset of states $|\alpha_{mn}\rangle$ form a complete set. Completeness is understood in the following sense: From $\langle\alpha_{mn}|f\rangle=0$ for all $|\alpha_{mn}\rangle$ it follows that $|f\rangle=0$. In Ref. 8 it was also proven that the set $|\alpha_{mn}\rangle$ is overcomplete by one state: that by removing any one state one obtains a strictly (or minimally) complete set of coherent states. The latter may be used as expansion basis for states and operators in quantum mechanics in a restricted sense.[8,9]

The nonorthogonality property is preserved by the set of states $|\alpha_{mn}\rangle$. Thus, for two coherent states $|\alpha\rangle$ and $|\beta\rangle$ one has[3]

$$\langle\beta|\alpha\rangle=\exp(-\tfrac{1}{2}|\alpha|^2-\tfrac{1}{2}|\beta|^2-\beta^*\alpha). \tag{4}$$

This relationship holds also for the states $|\alpha_{mn}\rangle$ with the replacement of α and β by their discrete values according to (3). It does not seem possible to modify the coherent states on a von Neumann lattice in such a way as to make them orthogonal.[10] Coherent states $|\alpha\rangle$ can be obtained from the ground state of a harmonic oscillator $|0\rangle$ by applying to it the displacement operator $D(\alpha)$ in the phase plane

$$|\alpha\rangle=D(\alpha)|0\rangle, \tag{5}$$

where

$$D(\alpha)=\exp(\alpha a^\dagger-\alpha^* a). \tag{6}$$

Correspondingly the states $|\alpha_{mn}\rangle$ are

$$|\alpha_{mn}\rangle=D(\alpha_{mn})|0\rangle. \tag{7}$$

It was shown in Ref. 10 that starting with any square-integrable state $|v\rangle$ one can generate a general von Neumann lattice of states according to the rule (7)

$$|v_{mn}\rangle=D(\alpha_{mn})|v\rangle. \tag{8}$$

The $|v_{mn}\rangle$, which we also call a von Neumann set, are not, in general, orthogonal. However, in Ref. 10 the class of $|v\rangle$, for which orthogonality does hold was

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found, and the $|v_{mn}\rangle$ turn out in this case to have the desirable property of forming a strictly complete orthogonal basis. But it was pointed out at the same time[10] that such states lose completely the semiclassical features of coherent states. Thus the product of uncertainties of $\hat{x}$ and $\hat{p}$ for them is $\Delta x \Delta p = \infty$. Since for coherent states $\Delta x \Delta p = \hbar/2$ it is impossible to convert them into an orthogonal von Neumann set without completely changing their classical character. Put in another way: states on a von Neumann lattice that posses coherence $\Delta x \Delta p < \infty$ are necessarily nonorthogonal. This striking opposition between desirable coherence properties and desirable completeness and orthogonality properties is one of the motives for studying general lattices of the type (8).

Having defined a von Neumann lattice of states, one can correspondingly define the amplitudes $\langle v_{mn} | f \rangle$ for an arbitrary $|f\rangle$ of the state space. Investigating different properties of these amplitudes will be the main subject of this paper. The investigation is carried out by establishing a close connection between the amplitudes $\langle v_{mn} | f \rangle$ of the state $|f\rangle$ and its kq-representation[11] $\langle k,q | f \rangle$. This connection is through the formula for the Fourier series expansion of the doubly periodic function $\langle v | k,q \rangle \langle k,q | f \rangle$, where $\langle k,q | v \rangle$ is the kq-representation of the generating state $|v\rangle$ for the lattice. The Fourier coefficients of this expansion are equal to $(-1)^{mn} \langle v_{mn} | f \rangle$. Thus for the coherent state lattice in particular, $(-1)^{mn} \langle \alpha_{mn} | f \rangle$ are the Fourier coefficients of $\langle 0 | k,q \rangle \langle k,q | f \rangle$, where $|0\rangle$ is the harmonic oscillator ground state. The quantities $(-1)^{mn} \langle \alpha_{mn} | 0 \rangle$ are therefore the Fourier coefficients of the probability density $|\langle k,q | 0 \rangle|^2$. Other cases of special interest are the lattices generated from the harmonic oscillator state $|N\rangle$.

$$|\alpha_{mn}^{(N)}\rangle = D(\alpha_{mn}) |N\rangle \tag{9}$$

[making a slight change of notation with respect to (8)]. The corresponding quantities $(-1)^{mn} \langle \alpha_{mn}^{(N)} | N \rangle$ are then the Fourier coefficients of the probability density $|\langle k,q | N \rangle|^2$.

The connection between the amplitudes $\langle v_{mn} | f \rangle$ and the kq-representation $\langle k,q | f \rangle$ for the state $|f\rangle$ turns out to be fruitful in establishing different properties of the $\langle v_{mn} | f \rangle$ and of the von Neumann set $\{|v_{mn}\rangle\}$. The most important of these are completeness and closure properties, the latter leading to some useful sum rules. We have mentioned that von Neumann lattices of states with coherence $\Delta x \Delta p < \infty$ are nonorthogonal sets. The Fourier expansion formula can be used to show in a simple way that any von Neumann set $\{|v_{mn}\rangle\}$ with coherence is not only nonorthogonal, but necessarily overcomplete (by one or more states), and also to obtain linear relationships between the amplitudes $\langle v_{mn} | f \rangle$ on such a lattice. In particular all the harmonic oscillator lattices $\{|\alpha_{mn}^{(N)}\rangle\}$ are overcomplete, not only the coherent state lattice. Therefore we can say that overcompleteness always accompanies coherence, which is a strengthening of the result of Ref. 10 that nonorthogonality always does so.

The same Fourier expansion formula is also used for finding closure relations for the $|v_{mn}\rangle$. For example, the sum of the squares of the amplitudes over the von Neumann lattice for any state $|f\rangle$,

$$\sum_{mn} |\langle v_{mn} | f \rangle|^2 , \tag{10}$$

can be evaluated explicitly from these closure relations. This sum may be compared with the corresponding sum for the amplitudes $\langle N | f \rangle$ with respect to the harmonic oscillator states (or any other orthonormal basis).

$$\sum_N |\langle N | f \rangle|^2 = \langle f | f \rangle . \tag{11}$$

It turns out, not unexpectedly, that only for orthogonal (and normalized) von Neumann sets does (10) sum as in (11) to $\langle f | f \rangle$ for all $|f\rangle$ in the state space. However, the explicit expressions for the sum (10) and other sum rules obtainable from the closure relations give us a great deal of further information. In particular, they will enable us to define a modified and enlarged Hilbert space of states in which the von Neumann set $|v_{mn}\rangle$ becomes strictly complete. As a by-product, they lead to a wealth of expressions for double sums. In the case of harmonic oscillator lattices, these expressions are relations among Laguerre polynomials, many of which do not seem to appear in the literature.

In Sec. II we shall deal only with the coherent state lattice as this is the most well known and important case. Then in Sec. III, which contains the main results, the discussion will be enlarged and extend to the general lattice of states (8). In Sec. IV the results are applied to lattices (9) of harmonic oscillator states. We conclude in Sec. IV. Appendix A contains some properties of the kq-representation wave functions used in the text, and Appendix B contains a discussion of the relationship between the Fourier expansion formula and the group theoretical properties of the displacements $D(\alpha_{mn})$ in (7).

II. VON NEUMANN LATTICE OF COHERENT STATES

Given a state $|\,\rangle$ in quantum-mechanics one can choose to express it in different representations.[12] Thus, $\langle x | \,\rangle$ is the Schrödinger representation of the state $|\,\rangle$. Similarly, one can write the expression $\langle \alpha | \,\rangle$ for this vector in the representation of coherent states. For a given vector $|f\rangle$ we shall use the following notation[2,3]:

$$\langle \alpha | f \rangle = \exp(-\tfrac{1}{2}|\alpha|^2) f(\alpha^*) , \tag{12}$$

where $f(\alpha^*)$ is known to be an entire function of α^*, the complex conjugate of α. [See Eq. (2)]. In particular, $\langle \alpha_{mn} | f \rangle$, the amplitude of the vector $|f\rangle$ on a von Neumann lattice, is

$$\langle \alpha_{mn} | f \rangle = \exp(-\tfrac{1}{2}|\alpha_{mn}|^2) f(\alpha_{mn}^*) . \tag{13}$$

This amplitude is a scalar product of the two vectors $|\alpha_{mn}\rangle$ and $|f\rangle$ and it assumes the following form in the x-representation[2]

$$\langle \alpha_{mn} | f \rangle = (-1)^{mn} \int \psi_0^*(x) \psi(x + na) \exp(-i(2\pi/a)xm)\, dx , \tag{14}$$

where $\psi_0(x)$ is the ground state of the harmonic oscillator and $\psi(x)$ is the x-representation of the state $|f\rangle$. To go over to the kq-representation we recall a few definitions.[11] The representation $\langle k,q | f \rangle$ of $|f\rangle$ is obtained from $\psi(x)$ by the transformation

$$\langle k,q|f\rangle=\left(\frac{a}{2\pi}\right)^{1/2}\sum_{s=-\infty}^{\infty}\exp(ikas)\psi(q-sa)\,. \qquad (15)$$

The formula (15) shows that a wave function in the kq-representation, $\langle k,q|f\rangle$ satisfies the following periodicity conditions[11]

$$\langle k+2\pi/a,q|f\rangle=\langle k,q|f\rangle\,, \qquad (16)$$

$$\langle k,q+a|f\rangle=\exp(ika)\langle k,q|f\rangle\,. \qquad (17)$$

The variables k,q are cyclic and their space of variation is the unit cell of the von Neumann lattice $0\leq q<a$, $0\leq k<2\pi/a$, also called the kq-cell. The state space consists therefore of functions $\langle k,q|f\rangle$ square integrable on the unit cell, and the scalar product of two states $|f\rangle$ and $|g\rangle$ is

$$\langle g|f\rangle=\int\langle g|k,q\rangle\langle k,q|f\rangle\,, \qquad (18)$$

where the integral is over the cell, and where $\langle g|k,q\rangle=\langle k,q|g\rangle^*$ as usual. Some properties of the functions $\langle k,q|f\rangle$ relevant to this paper are given in Appendix A.

The harmonic oscillator ground state $|0\rangle$ has the kq-representation

$$\langle k,q|0\rangle=\left(\frac{a}{2\pi^{3/2}\lambda}\right)^{1/2}\sum_{s=-\infty}^{\infty}\exp\left(ikas-\frac{(q-sa)^2}{2\lambda^2}\right). \qquad (19)$$

It was previously shown[10] that the states $|\alpha_{mn}\rangle$ assume a canonical form in the kq-representation

$$\langle k,q|\alpha_{mn}\rangle=(-1)^{mn}\exp(i(2\pi/a)qm-iakn)\langle k,q|0\rangle\,. \qquad (20)$$

The amplitude (14) can therefore be written via the scalar product formula (18) as

$$\langle\alpha_{mn}|f\rangle=(-1)^{mn}\int\langle 0|k,q\rangle\langle k,q|f\rangle\exp(-i(2\pi/a)qm+iakn)\times dk\,dq\,. \qquad (21)$$

Now it follows from the periodicity conditions (16) and (17) that any product of wave functions $\langle k,q|f\rangle$ and $\langle k,q|g\rangle$ in the form

$$\langle g|k,q\rangle\langle k,q|f\rangle \qquad (22)$$

is strictly periodic in both variables k and q. Therefore the amplitudes $\langle\alpha_{mn}|f\rangle$ in (21) can be interpreted in the following way: $(-1)^{mn}\langle\alpha_{mn}|f\rangle$ are the Fourier coefficients of the periodic function $\langle 0|k,q\rangle\langle k,q|f\rangle$. We have arrived therefore at the basic formula connecting the amplitudes $\langle\alpha_{mn}|f\rangle$ of any state $|f\rangle$ on the coherent state von Neumann lattice with the wave function $\langle k,q|f\rangle$: the Fourier expansion

$$\langle 0|k,q\rangle\langle k,q|f\rangle=\frac{1}{2\pi}\sum_{mn}(-1)^{mn}\langle\alpha_{mn}|f\rangle\exp\left(i\frac{2\pi}{a}qm-iakn\right). \qquad (23)$$

It is important, for later discussion, to underline that the equivalence in (23) is strictly that of Fourier series, and pointwise convergence in the kq-cell does not always hold.[13] Let us denote the expanded function by

$$F(k,q)\equiv\langle 0|k,q\rangle\langle k,q|f\rangle\,. \qquad (24)$$

Since $\langle 0|k,q\rangle$ is a fixed function it follows that Eq. (24) defines a correspondence between any state $|f\rangle$ and the periodic function $F(k,q)$. It is clear that if $\langle k,q|f\rangle$ is a square-integrable function then also $F(k,q)$ is square integrable. This follows from the fact that the fixed function $\langle k,q|0\rangle$ in (24) is smooth. The latter can also be written in the following way[9]:

$$\langle k,q|0\rangle=(a/2\pi^{3/2}\lambda)^{1/2}\exp(-q^2/2\lambda^2)\Theta_3(z|\tau)\,, \qquad (25)$$

with $z=\frac{1}{2}ka-(i/2)(aq/\lambda^2)$. In (25) $\Theta_3(z|\tau)$ is the theta function[14] which is an entire function of the variable z and has one simple zero at $z_0=\pi/2-ia^2/4\lambda^2$ in a unit cell of the von Neumann lattice; the parameter $\tau=ia^2/2\pi\lambda^2$. Equation (24) gives therefore a square-integrable periodic function $F(k,q)$ for every square-integrable state $|f\rangle$.

Let us return to the interpretation of the Fourier expansion (23). On the left-hand side we have the periodic function $\langle 0|k,q\rangle\langle k,q|f\rangle$. Such a product can appear in physical expressions when one takes the square of the absolute value of the vector $(|0\rangle+|f\rangle)$ in the kq-representation. This square will contain the terms $|\langle k,q|0\rangle|^2$, $|\langle k,q|f\rangle|^2$, and the cross or interference term $\langle 0|k,q\rangle\langle k,q|f\rangle$. The left-hand side of the expansion (23) can therefore be given the meaning of an interference term and we arrive at the following interpretation: $(-1)^{mn}\langle\alpha_{mn}|f\rangle$ are the Fourier coefficients of the interference term $\langle 0|k,q\rangle\langle k,q|f\rangle$ in the superposition of the states $|0\rangle$ and $|f\rangle$. In the particular, case when $|f\rangle=|0\rangle$, Eq. (23) assumes the form

$$F_0(k,q)=|\langle k,q|0\rangle|^2=\frac{1}{2\pi}\sum_{m,n}(-1)^{mn}\langle\alpha_{mn}|0\rangle\times\exp\left(i\frac{2\pi}{a}qm-iakn\right), \qquad (26)$$

where the subscript 0 denotes the ground state. In this case the left-hand side has the meaning of a probability density distribution for the ground state of a harmonic oscillator. Correspondingly, $(-1)^{mn}\langle\alpha_{mn}|0\rangle$ are its Fourier coefficients. This means that the amplitudes $\langle\alpha_{mn}|0\rangle$ can directly be obtained by Fourier analyzing the probability density $F_0(k,q)$.

Equation (26) can be written in an explicit form by using the expression $\langle\alpha_{mn}|0\rangle=\exp(-\frac{1}{2}|\alpha_{mn}|^2)$ found from (4), and the definition for α_{mn} in Eq. (3). We have

$$F_0(k,q)=\frac{1}{2\pi}\sum_{m,n}(-1)^{mn}\exp\left\{-\frac{a^2}{4\lambda^2}\left[n^2+\left(\frac{2\pi}{a^2}\lambda^2\right)^2m^2\right]\right\}\times\exp\left(i\frac{2\pi}{a}qm-iakn\right). \qquad (27)$$

This is an expression for the ground state probability density as a function of k and q. It assumes a very simple form for the symmetric case, when $(2\pi/a^2)\lambda^2=1$. When this condition holds, the expression (27) assumes a fully symmetric form

$$F_0(k,q)=\frac{1}{2\pi}\sum_{m,n}(-1)^{mn}\exp\left(-\frac{\pi}{2}(n^2+m^2)\right)\times\exp\left(i\frac{2\pi}{a}qm-iakn\right). \qquad (28)$$

An another example, let us consider the case when $|f\rangle = |N\rangle$, where $|N\rangle$ is the Nth harmonic oscillator state. In this case we have

$$F_N(k,q) \equiv \langle 0|k,q\rangle\langle k,q|N\rangle = \frac{1}{2\pi}\sum(-1)^{mn}\frac{(\alpha^*_{mn})^N}{\sqrt{N!}}\exp(-\tfrac{1}{2}|\alpha_{mn}|^2) \times\exp\left(i\frac{2\pi}{a}qm - iakn\right), \tag{29}$$

where we used the expression[3]

$$\langle\alpha_{mn}|N\rangle = \frac{(\alpha^*_{mn})^N}{\sqrt{N!}}\exp(-\tfrac{1}{2}|\alpha_{mn}|^2). \tag{30}$$

The formula (29) goes over into (26) when $N=0$.

Let us consider the case, $|f\rangle = |\alpha\rangle$, where $|\alpha\rangle$ is a coherent state. Using the formula [from (4)]

$$\langle\alpha_{mn}|\alpha\rangle = \exp(-\tfrac{1}{2}|\alpha_{mn}|^2 - \tfrac{1}{2}|\alpha|^2 + \alpha^*_{mn}\alpha), \tag{31}$$

we find from (23)

$$F_\alpha(k,q) \equiv \langle 0|k,q\rangle\langle k,q|\alpha\rangle = \frac{1}{2\pi}\sum_{m,n}(-1)^{mn}\exp(-\tfrac{1}{2}|\alpha|^2 - \tfrac{1}{2}|\alpha_{mn}|^2 + \alpha^*_{mn}\alpha) \times\exp\left(i\frac{2\pi}{a}qm - iakn\right). \tag{32}$$

The functions on the left-hand sides in (26), (29), and (32) are continuous with continuous derivatives of any order. Therefore their Fourier expansions converge to them uniformly in the variables k and q and the left- and right-hand sides can be equated at every point.[13] Thus, if we assume in (32) $k=\pi/a, q=a/2$, the left-hand side of this relation vanishes (this point is the zero of the function $\langle 0|k,q\rangle$) and we arrive at the following identity for any α:

$$\sum_{mn}(-1)^{mn+m+n}\exp(-\tfrac{1}{2}|\alpha_{mn}|^2 + \alpha^*_{mn}\alpha) = 0. \tag{33}$$

This identity was already obtained by Perelomov by other means.[8] It can immediately be generalized for any state $|f\rangle$ with the property that $\langle k,q|f\rangle$ is a function whose second derivatives exist and are square integrable. For such a function $\langle k,q|f\rangle$, the function $F(kq)$ in (24) will also satisfy the same conditions, and therefore from the theory of Fourier series it follows that Eq. (23) will converge uniformly in k and q.[13,15] Thus at $k=\pi/a, q=a/2$ we find a generalization of (33)

$$\sum_{mn}(-1)^{mn+m+n}\langle\alpha_{mn}|f\rangle = 0, \quad (|f\rangle \text{ in } \mathfrak{D}). \tag{34}$$

Here we have denoted by $\mathfrak{D}$ the class of functions with the property mentioned above. Certainly (34) holds for a larger class of functions than $\mathfrak{D}$ because it is known that in (23) convergence at $k=\pi/a, q=a/2$ is assured whenever the function is sufficiently regular around that point. However, whether or not the linear relationship holds for any square-integrable state $|f\rangle$ without restriction, remains an open question. In any case, (34) shows that the amplitudes $\langle\alpha_{mn}|f\rangle$ turn out to be linearly dependent for an important class of $|f\rangle$, a class that is in fact dense in the state space. This is certainly a consequence of the overcompleteness of the set $|\alpha_{mn}\rangle$ mentioned above. We have emphasized the domain $\mathfrak{D}$ in (34) because it is a very distinguished one in the state space. Let us recall that the position and momentum operators are given in the kq-representation by[11]

$$\hat{x} = q + i\frac{\partial}{\partial k}; \quad \hat{p} = -i\frac{\partial}{\partial q}. \tag{35}$$

The domain $\mathfrak{D}$ of functions $\langle k,q|f\rangle$ consists therefore precisely of those on which not only $\hat{x}$ and $\hat{p}$ but also $\hat{x}^2$, $\hat{p}^2$ and $\hat{x}\hat{p}, \hat{p}\hat{x}$ are defined. In other words they are just the states which possess the coherence property $\Delta x\Delta p < \infty$ and for which the correlations $\overline{xp}$ and $\overline{px} = \overline{xp} - i\hbar$ are also finite.

The Fourier expansion (23) can be used directly for checking the completeness of the set $|\alpha_{mn}\rangle$ of coherent states.[7,8,10] One can obtain an entirely elementary proof that the set of $|\alpha_{mn}\rangle$ with one state removed is a strictly complete set for square-integrable states $|f\rangle$. Since this feature of the set $|\alpha_{mn}\rangle$ is so striking and since the proof is so simple we shall give it here again.

In the first place, it follows immediately from (23) that the square-integrable function $\langle 0|k,q\rangle\langle k,q|f\rangle$ is zero if all its coefficients $\langle\alpha_{mn}|f\rangle = 0$. Since $\langle 0|k,q\rangle$ has only one zero in a unit cell of the von Neumann lattice [see Eq. (25)] it follows also that $\langle k,q|f\rangle$ is zero almost everywhere. This proves that the set $|\alpha_{mn}\rangle$ for all α_{mn} is complete. Assume now, that $\langle\alpha_{mn}|f\rangle = 0$ for all α_{mn} but one, say α_{rs}. Then from (23) it follows

$$\langle 0|k,q\rangle\langle k,q|f\rangle = [(-1)^{rs}/2\pi]\langle\alpha_{rs}|f\rangle \times\exp(i(2\pi/a)qr - iaks).$$

Since the function $\langle 0|k,q\rangle$ has a zero [see Eq. (25)] it follows that also $\langle\alpha_{rs}|f\rangle$ has to be zero otherwise $\langle k,q|f\rangle$ would not be a square-integrable function, contrary to the above assumption. We conclude therefore that if $\langle\alpha_{mn}|f\rangle = 0$ for all α_{mn} but one, then necessarily $\langle k,q|f\rangle$ is zero almost everywhere. This proves that the set $|\alpha_{mn}\rangle$ with one state removed, say $|\alpha_{rs}\rangle$ and $|\alpha_{tu}\rangle$ then the remaining set is no longer complete. To prove this, assume that $\langle\alpha_{mn}|f\rangle = 0$ for all α_{mn} but α_{rs} and α_{tu}. From the Fourier expansion (23) we have

$$\langle k,q|f\rangle = (1/2\pi)\langle 0|k,q\rangle^{-1}[(-1)^{rs}\langle\alpha_{rs}|f\rangle \times\exp(i(2\pi/a)qr - iaks) + (-1)^{tu}\langle\alpha_{tu}|f\rangle\exp(i(2\pi/a)qt - iaku)]. \tag{36}$$

To show that the set $|\alpha_{mn}\rangle$ with the two states $|\alpha_{rs}\rangle$ and $|\alpha_{tu}\rangle$ removed is no longer complete it is sufficient to show that the coefficients $\langle\alpha_{rs}|f\rangle$ and $\langle\alpha_{tu}|f\rangle$ in the above function can be chosen in such a way as to make it square integrable. This is achieved if we demand that the right-hand side of (36) vanish at the same point $k=\pi/a, q=a/2$, that $\langle k,q|0\rangle$ does. Assume therefore the condition

$$(-1)^{rs+r+s}\langle\alpha_{rs}|f\rangle + (-1)^{tu+t+u}\langle\alpha_{tu}|f\rangle = 0. \tag{37}$$

With this condition the function (36) is square integrable which means that $\langle\alpha_{mn}|f\rangle = 0$ for all α_{mn} but α_{rs} and α_{tu} does not lead to $|f\rangle \equiv 0$. The set $|\alpha_{mn}\rangle$ with one state removed is strictly complete with respect to the space of square-integrable states $|f\rangle$. Although this formal result is by now well established, its physical meaning is far from being clear. From the point of view of the physical structure of von Neumann lattices with a unit cell area of h the removal of one state is not demanded by any physical intuition. It is therefore of interest to find out how to enlarge the space of functions in order to make the full set $|\alpha_{mn}\rangle$ complete. We return to this below.

We can exploit further properties of the Fourier expansion (23) to derive closure relations and sum rules for the amplitudes $\langle\alpha_{mn}|f\rangle$. We have seen that the function $\langle 0|k,q\rangle\langle k,q|f\rangle$ of (23) is not only integrable but square integrable as well for all $|f\rangle$. There are some well-known rules for the Fourier coefficients of square integrable functions (Ref. 13, p. 248). If c_{mn} are the Fourier coefficients of a doubly-periodic square integrable function $\varphi(k,q)$, then

$$\sum_{mn} |c_{mn}|^2 = 2\pi \int |\varphi(k,q)|^2 \, dk\, dq , \tag{38}$$

c_{mn} and c'_{mn} are the Fourier coefficients of two different square-integrable functions, $\varphi(k,q)$ and $\varphi'(k,q)$, respectively, then

$$\sum_{mn} c_{mn} c'_{mn} = 2\pi \int \varphi^*(k,q) \quad \varphi'(k,q)\, dk\, dq , \tag{39}$$

Applying (38) and (39) to the expansions (23) we arrive at the closure relations in the form of sum rules for the amplitudes $\langle\alpha_{mn}|f\rangle$

$$\sum_{mn} |\langle\alpha_{mn}|f\rangle|^2 = \int |\langle k,q|0\rangle|^2 |\langle k,q|f\rangle|^2 \, dk\, dq \tag{40}$$

for any state $|f\rangle$ and

$$\sum_{mn} \langle g|\alpha_{mn}\rangle\langle\alpha_{mn}|f\rangle = \int |\langle k,q|0\rangle|^2 \langle g|k,q\rangle\langle k,q|f\rangle \, dk\, dq \tag{41}$$

for any two states $|f\rangle$ and $|g\rangle$. The relations (40) and (41) are interesting in several respects. They not only show that the sum of the squares of the amplitudes is always bounded [which could have been deduced from (14)], but they give explicit expressions for them in a new form. Another aspect of (40) and (41) is that they tell us directly how we may enlarge the space so that the set $|\alpha_{mn}\rangle$ becomes strictly complete. We define a modified Hilbert space, which includes the original one, by taking the right-hand side of (40) and (41) to be a new norm and scalar product, respectively. Thus a function belongs to the modified space wherever the integral (40) with weight function $|\langle k,q|0\rangle|^2$ is finite. It is not hard then to see from (40) that the new space has nonvanishing functions for which $\langle\alpha_{mn}|f\rangle = 0$ for all except one member of the lattice. We discuss this question in more detail for general lattices in the next section. Although there is a more satisfying symmetry with respect to the von Neumann lattice in the modified space, the full physical meaning of the weighted norm remains unclear.

III. VON NEUMANN LATTICES OF ARBITRARY STATES

The results of the previous section can straightforwardly be formulated for von Neumann lattices of arbitrary states. As was shown in Ref. 10, given an arbitrary state $|v\rangle$ one obtains a discrete set of states by displacing it according to Eq. (8). Having this in mind one can derive the main Fourier expansion formula [Eq. (23)] for any set of states $|v_{mn}\rangle$ on a von Neumann lattice.

As in the coherent state case the $|v_{mn}\rangle$ assume a simple form in the kq-representation

$$\langle k,q|v_{mn}\rangle = (-1)^{mn} \exp(i(2\pi/a)qm - iakn)\langle k,q|v\rangle , \tag{42}$$

where $\langle k,q|v\rangle$ is the wave function for the generating state $|v\rangle$. The amplitudes of any state $|f\rangle$ on the von Neumann lattice of states $|v_{mn}\rangle$ are, using (18),

$$\langle v_{mn}|f\rangle = (-1)^{mn} \int \langle v|k,q\rangle\langle k,q|f\rangle \exp(-i(2\pi/a)qm + iakn) \times dk\, dq , \tag{43}$$

and therefore the basic Fourier expansion formula is

$$\langle v|k,q\rangle\langle k,q|f\rangle = \frac{1}{2\pi}\sum_{mn} (-1)^{mn}\langle v_{mn}|f\rangle \times \exp\left(i\frac{2\pi}{a}qm - iakn\right) \tag{44}$$

in exact analogy to (23). Thus the amplitude $\langle v_{mn}|f\rangle$ has the following interpretation: $(-1)^{mn}\langle v_{mn}|f\rangle$ are the Fourier coefficients of the interference term $\langle v|k,q\rangle \times \langle k,q|f\rangle$ in the superposition of the states $|v\rangle$ and $|f\rangle$. The function $\langle v|k,q\rangle\langle k,q|f\rangle$ is clearly strictly periodic in both variables from (16) and and (17). For $|f\rangle = |v\rangle$, in particular,

$$|\langle v|k,q\rangle|^2 = \frac{1}{2\pi}\sum_{mn} (-1)^{mn}\langle v_{mn}|v\rangle \exp\left(i\frac{2\pi}{a}qm - iakn\right). \tag{45}$$

Thus we have a connection between the probability density for an arbitrary vector $|v\rangle$ in the kq-cell and its amplitudes on its own von Neumann lattice.

Equation (44) is the key formula in the study of the von Neumann set $\{|v_{mn}\rangle\}$. In Appendix B we show that it has a deeper significance in terms of the group properties of the phase-space displacements $D(\alpha_{mn})$. Essentially all the properties of the $|v_{mn}\rangle$ derived below follow from the nature of (44) as a Fourier series expansion [c.f., observation under Eq. (23)].

As a first remark, we note that the set of $|v_{mn}\rangle$ is incomplete if the generating state $|v\rangle$ has a wave function $\langle k,q|v\rangle$ that vanishes on a set of finite measure in the kq-cell. Because even if all amplitudes $\langle v_{mn}|f\rangle$ vanish, so that the left-hand side of (44) is the zero function, we cannot conclude that $\langle k,q|f\rangle$ it itself zero. This repeats a result of Ref. 10. From now on we exclude such $|v\rangle$ as generating states, so that the $|v_{mn}\rangle$ will always be complete. It will turn out that in a large class of important cases they are overcomplete, as for the coherent state lattice.

We shall make another restriction on the generating state $|v\rangle$: we suppose that in (44) the function $\langle v|k,q\rangle \times \langle k,q|f\rangle$ is square integrable for all square-integrable $\langle k,q|f\rangle$. This would certainly not be true for arbitrary $|v\rangle$ but it does hold for "reasonable" $|v\rangle$ and we want to exclude pathological cases. It holds, in particular, for those $|v\rangle$, like $|0\rangle$ or $|N\rangle$, that possess the coherence property $\Delta x \Delta p < \infty$ and belong to the class denoted by $\mathfrak{D}$ in Sec. II. This is because the $\langle k,q|v\rangle$ are smooth enough. It also holds for the cases where the von Neumann set $|v_{mn}\rangle$ is an orthogonal one. Because here the function $\langle k,q|v\rangle$ has the property $|\langle k,q|v\rangle| \equiv$ constant.[10] We can see this from (18) and (42), or directly from (45). At first sight the latter kind of lattice seems to be the most desirable one for a quantum-mechanical representation based on the set of amplitudes $\langle v_{mn}|f\rangle$, because the $|v_{mn}\rangle$ form a strictly complete orthogonal basis. The snag is that, as mentioned in the Introduction, the orthogonal $|v_{mn}\rangle$ lose all coherence properties: in other words $|v\rangle$ cannot be in the class . The proof of this is repeated in Appendix A and is based on the following remarkable property of the kq-representation[16,17]: If for a state $|v\rangle$ the wave function $\langle k,q|v\rangle$ is continuous in the variables k and q, then the periodicity conditions (16) and (17) force $\langle k,q|v\rangle$ to vanish at least at one point in the kq-cell. Clearly then the twice-differentiable functions of $\mathfrak{D}$ cannot satisfy $|\langle k,q|v\rangle| \equiv C > 0$.

Let us return to the Fourier expansion (44), and suppose now that $|v\rangle$ belongs to the physically interesting class $\mathfrak{D}$. The fact that $\langle k,q|v\rangle$ vanishes at some points can be used to prove in an entirely elementary way that the set $\{|v_{mn}\rangle\}$ is necessarily overcomplete. It can be carried out in much the same way as for the $|\alpha_{mn}\rangle$. To find the degree of overcompleteness, however, we need more information about the zeros of $\langle k,q|v\rangle$. For example, for the $|\alpha_{mn}\rangle$, we explicitly used the fact that $\langle k,q|0\rangle$ has one zero in the unit cell to show that the set was overcomplete by one state. This can be generalized: in a separate publication it will be shown that if $\langle k,q|v\rangle$ has, say, r simple zeros then the $|v_{mn}\rangle$ are overcomplete by r members.

Although, when the number of zeros is finite, the set can be made strictly complete by removing a finite number of members, the question of whether and how the remaining $|v_{mn}\rangle$ can be used as a basis for expansions of general states $|f\rangle$ is a more subtle and apparently more difficult one. Apart from the rather arbitrary way in which we can select the states for removal, there are many further problems with expanding in nonorthogonal bases.[18] For the coherent state lattice, the problems have been discussed elsewhere.[8,9] These difficulties are one reason why we indicate below that it is possible to construct a modified Hilbert space in which the $|v_{mn}\rangle$ become strictly complete.

The overcompleteness gives rise to linear dependencies among the amplitudes $\langle v_{mn}|f\rangle$ of a type similar to (34). If $|f\rangle$ as well as $|v\rangle$ belongs to $\mathfrak{D}$, then the Fourier series expansion (44) converges uniformly in the variables k and q.[13,15] Suppose k_0, q_0 is a point at which $\langle k_0,q_0|v\rangle = 0$; then from (44)

$$\sum_{mn} (-1)^{mn} \exp\left(i\frac{2\pi}{a}q_0 m - iak_0 n\right)\langle v_{mn}|f\rangle = 0 \quad (|v\rangle,\ |f\rangle \text{ in } \mathfrak{D}). \tag{46}$$

As with Eq. (34), it is not clear whether, for a fixed lattice, this can be extended to all $|f\rangle$ in the state space. In any case (46) yields some interesting double sum identities in the special case $|v\rangle = |V\rangle$ (Sec. IV).

We now derive a set of sum rules for the amplitudes $\langle v_{mn}|f\rangle$ based on the fact that the function expanded in (44) is square integrable (by assumption). In exactly the same manner as for (40) and (41), we can show from (38) and (39) that for any states $|f\rangle$ and $|g\rangle$

$$\sum_{mn} |\langle v_{mn}|f\rangle|^2 = \int |\langle k,q|v\rangle^2|\langle k,q|f\rangle|^2\,dk\,dq\,, \tag{47}$$

$$\sum_{mn} \langle g|v_{mn}\rangle\langle v_{mn}|f\rangle = \int |\langle k,q|v\rangle|^2\langle g|k,q\rangle\langle k,q|f\rangle\,dk\,dq\,. \tag{48}$$

These sums are clearly always finite for the lattices under consideration. They can be summarized in a compact form by the closure relation

$$\sum_{mn} |v_{mn}\rangle\langle v_{mn}| = \sum_{mn} \langle v_{mn}|v\rangle D(\alpha_{mn})\,. \tag{49}$$

This is proved by substituting in (48) the expression for $|\langle v|k,q\rangle|^2$ from (45) and using (42) and (8); one then easily verifies that (48) is a matrix element of (49). Equation (49) can be further generalized to give a quite useful identity. Suppose $|v\rangle$ and $|w\rangle$ are generating functions for two different von Neumann lattices of states. Equations (38) and (39) can again be used with (44) to show that

$$\sum_{mn} |v_{mn}\rangle\langle w_{mn}| = \sum_{mn} \langle w_{mn}|v\rangle D(\alpha_{mn})$$

from which we derive, in particular, the sum rule

$$\sum_{mn} \langle v|v_{mn}\rangle\langle w_{mn}|w\rangle = \sum_{mn} |\langle w_{mn}|v\rangle|^2\,. \tag{50}$$

This will be used in Sec. IV.

The sum rules (47) and (48), or alternatively the closure relation (49), differ of course from the corresponding ones for amplitudes on orthonormal bases like (11). One obtains indeed

$$\sum_{mn} |\langle v_{mn}|f\rangle|^2 = \langle f|f\rangle$$

for all $|f\rangle$, or equivalently

$$\sum_{mn} |v_{mn}\rangle\langle v_{mn}| = I \quad \text{(unit operator)}$$

only when $|\langle k,q|v\rangle|^2 \equiv 1$, as may be seen from (47). This of course, is when the $|v_{mn}\rangle$ form a complete orthonormal basis.

In general, if $|v\rangle$ is normalized the first term in (49) is I and the remainder measures the departure from strict closure. For the coherent state lattice, for instance, (49) is

$$\sum_{mn} |\alpha_{mn}\rangle\langle\alpha_{mn}| = \sum_{mn} \exp(-\tfrac{1}{2}|\alpha_{mn}|^2) D(\alpha_{mn})\,, \tag{51}$$

since $\langle\alpha_{mn}|0\rangle = \exp(-\frac{1}{2}|\alpha_{mn}|^2)$. It is interesting to compare (51) with the decomposition of unity for the full set of coherent states[3]

$$\frac{1}{2\pi\hbar}\int |\alpha\rangle\langle\alpha|\, d\bar{x}\, d\bar{p}=I\,,$$

where $\bar{x}$ and $\bar{p}$ are defined in (2). Integration over the whole phase space with density function $(d\bar{x}\,d\bar{p})/2\pi\hbar$ gives the unit I, whereas for the discrete sum (51) over the von Neumann lattice the result differs from I.

Another virtue of the sum rules (47) and (48) is that they give us the solution to the following problem: What is the space of functions for which the $|v_{mn}\rangle$ become strictly complete, i.e., where there are no redundant amplitudes $\langle v_{mn}|f\rangle$? The answer is: the Hilbert space of functions $\langle k,q|f^*\rangle$ for which the weighted norm on the right-hand side of (47) is finite. The corresponding scalar product is given by the right-hand side of (48). We have introduced the asterisk in $|f^*\rangle$ because the modified Hilbert space is, in general, larger than the original one. The $\langle k,q|f^*\rangle$ are characterized by

$$\langle k,q|f^*\rangle = F(k,q)/\langle v|k,q\rangle\,, \tag{52}$$

where the $F(k,q)$ are strictly periodic and square integrable. If $\langle v|k,q\rangle$ has zeros, there clearly exist $\langle k,q|f^*\rangle$ outside the usual space. Let us consider the von Neumann set $|v^*_{mn}\rangle$ generated from $|v^*\rangle$ in the usual way with

$$\langle k,q|v^*\rangle = 1/\langle v|k,q\rangle\,. \tag{53}$$

Then from (47), the $|v^*_{mn}\rangle$ are a complete orthonormal basis of the modified space. Any $|f^*\rangle$ can be expanded uniquely in this basis and it is easy to check from (42), (48), and (53) that the expansion coefficients are equal to the amplitudes $\langle v_{mn}|f^*\rangle$. Hence from the strict completeness of the $|v^*_{mn}\rangle$ follows the strict completeness of $|v_{mn}\rangle$.

We arrive, therefore, at the intriguing conclusion, that if we are ready to enlarge the space of physical states to those $\langle k,q|f^*\rangle$ for which $F(k,q)$ is square integrable in (52), then we remove the awkwardness of overcompleteness. We have particularly in mind the coherent state lattice, where the necessity of removing one state from the set does not seem to have a simple physical interpretation. On the other hand, although in the modified space the role of the underlying unit cell of area h is more sharply outlined, the physical meaning of the new norm, weighted by $|\langle v|k,q\rangle|^2$, remains unclear.

IV. LATTICES OF HARMONIC STATES

Von Neumann lattices generated from harmonic oscillator states $|N\rangle$ are the natural generalization of the coherent state lattice. Apart from their intrinsic interest, their study leads to an almost embarrassing wealth of relationships for double sums, obtained by applying the formulas of Sec. III. Some of them, at least, appear to be new.

The lattice of states $|\alpha^{(N)}_{mn}\rangle$ generated from $|N\rangle \equiv |\alpha^{(N)}_{00}\rangle$, defined in (9), has the Fourier expansion formula (44)

$$\langle N|k,q\rangle\langle k,q|f\rangle = \frac{1}{2\pi}\sum_{mn}(-1)^{mn}\langle\alpha^{(N)}_{mn}|f\rangle\exp\left(i\frac{2\pi}{a}qm - iakn\right). \tag{54}$$

The wave function $\langle k,q|N\rangle$ is calculated from (15) with $\psi(x)=u_N(x)$, the normalized Hermite function of order N. It can be shown that $\langle k,q|N\rangle$ is a smooth, in fact analytic, function of the variables k and q. This ensures that it can vanish only on a set of zero measure in the kq-cell. Since it belongs *a fortiori* to the class $\mathfrak{D}$ of Sec. II, on the other hand, we know from the discussion in the last section that it does possess zeros. In fact, from that discussion we know (i) that the set $|\alpha^{(N)}_{mn}\rangle$ is complete for any N, (ii) that it is always overcomplete by at least one member, and (iii) that for an $|f\rangle$ of class $\mathfrak{D}$ the sum (54) converges uniformly in k and q.

For the case $N=0$, we know from (25) that the degree of overcompleteness is just one (Sec. II); but for $N>0$ the number and location of the zeros of $\langle k,q|N\rangle$ is as yet a not completely solved problem. However, it is not difficult to verify from (15) that when $\psi(x)$ is even in x, there is a zero at $k=\pi/a, q=a/2$; and that when $\psi(x)$ is odd there are zeros at $k=0,\ q=0;\ k=\pi/a$, and $k=0$, $q=a/2$ (see Appendix A). Thus for N odd, overcompleteness is by at least three members.

Important special cases of (54) are for $|f\rangle$ itself a harmonic oscillator state

$$\langle N|k,q\rangle\langle k,q|M\rangle = \frac{1}{2\pi}\sum_{mn}(-1)^{mn}\langle\alpha^{(N)}_{mn}|M\rangle\exp\left(i\frac{2\pi}{a}qm - iakn\right), \tag{55}$$

$$|\langle N|k,q\rangle|^2 = \frac{1}{2\pi}\sum_{mn}(-1)^{mn}\langle\alpha^{(N)}_{mn}|N\rangle\exp\left(i\frac{2\pi}{a}qm - iakn\right). \tag{56}$$

The coefficients $\langle\alpha^{(N)}_{mn}|M\rangle$ are known[4]

$$\langle M|\alpha^{(N)}_{mn}\rangle = \begin{cases}\exp(-\frac{1}{2}|\alpha_{mn}|^2)\alpha_{mn}^{M-N}\sqrt{N!/M!}\,L_N^{M-N}(|\alpha_{mn}|^2), & M\geq N\\ \exp(-\frac{1}{2}|\alpha_{mn}|^2)(-\alpha^*_{mn})^{N-M}\sqrt{M!/N!}\,L_M^{N-M}(|\alpha_{mn}|^2), & M\leq N\end{cases}, \tag{57}$$

where $L_N^M(x)$ is a Laguerre polynomial[19] ($L_N^0(x)\equiv L_N(x)$).

Equations (55) and (56) for the interference term and probability density for harmonic oscillator wave functions in the kq-representation clearly generalize (26) and (29). Using our knowledge of the location of some of the zeros, and remark (iii) above, we find some interesting relationships of the type (46). Thus using (57) in (56) we get four relationships from the known zeros, of which we exhibit two

$$\sum_{mn}(-1)^{mn}\exp(-\tfrac{1}{2}|\alpha_{mn}|^2)L_N(|\alpha_{mn}|^2)=0 \quad (N \text{ odd})$$
$$\sum_{mn}(-1)^{m+n+mn}\exp(-\tfrac{1}{2}|\alpha_{mn}|^2)L_N(|\alpha_{mn}|^2)=0 \quad (N \text{ even}). \tag{58}$$

More are obtainable by taking different combinations of odd/even for M/N in (55). Thus for example suppose N even and M arbitrary $> N$: one finds

$$\sum_{mn} (-1)^{mn+m+n} \exp(-\tfrac{1}{2}|\alpha_{mn}|^2)\alpha_{mn}^{M-N} L_N^{M-N}(|\alpha_{mn}|^2) = 0 \qquad (M > N;\ N \text{ even}). \qquad (58')$$

This is a direct generalization of the sums discovered by Perelomov[8] for the case $N=0$:

$$\sum_{mn} (-1)^{mn+m+n} \exp(-\tfrac{1}{2}|\alpha_{mn}|^2)\alpha_{mn}^{M} = 0$$

[where we use $L_0^M(x) \equiv 1$].

Let us now consider some examples of the sum rules (47)–(50) applied here; all the conditions to do so are fulfilled. From (47) we get

$$\sum_{mn} |\langle \alpha_{mn}^{(N)} | f\rangle|^2 = \int |\langle k,q|N\rangle|^2 |\langle k,q|f\rangle|^2 \, dk\, dq\,, \qquad (59)$$

which generalizes (40) for the coherent state case; and from (49) and (57) we obtain as a generalization of (51) the closure relation

$$\sum_{mn} |\alpha_{mn}^{(N)}\rangle\langle \alpha_{mn}^{(N)}| = \sum_{mn} \exp(-\tfrac{1}{2}|\alpha_{mn}|^2) L_N(|\alpha_{mn}|^2) D(\alpha_{mn})\,. \qquad (60)$$

The identity (50) yields some very interesting relations. Take $|v\rangle = |M\rangle$ and $|w\rangle = |N\rangle$

$$\sum_{mn} \langle M|\alpha_{mn}^{(M)}\rangle\langle \alpha_{mn}^{(N)}|N\rangle = \sum_{mn} |\langle \alpha_{mn}^{(N)}|M\rangle|^2\,. \qquad (61)$$

Using (57) and supposing for definiteness that $M > N$

$$\sum_{mn} \exp(-|\alpha_{mn}|^2) L_M(|\alpha_{mn}|^2) L_N(|\alpha_{mn}|^2) = \frac{N!}{M!} \sum_{mn} \exp(-|\alpha_{mn}|^2) |\alpha_{mn}|^{2(M-N)} [L_N^{M-N}(|\alpha_{mn}|^2)]^2\,. \qquad (62)$$

These relations between Laguerre polynomials of different orders appear to be new, in their general form. Let us consider the simple case when $M=1, N=0$. From (62) we find, having in mind that[19] $L_0(x)=1$, $L_1(x) = 1-x$ and $L_0 = 1$:

$$2\sum_{m,n} \exp(-|\alpha_{mn}|^2)|\alpha_{mn}|^2 = \sum_{m,n} \exp(-|\alpha_{mn}|^2)\,. \qquad (63)$$

For the symmetric case, when $(2\pi/a^2)\lambda^2 = 1$ [see also Eq. (28)], (63) becomes

$$2\pi \sum_{m,n} (m^2+n^2) \exp[-\pi(m^2+n^2)] = \sum_{m,n} \exp[-\pi(m^2+n^2)]\,, \qquad (64)$$

which also reduces to

$$4\pi \sum_{m=-\infty}^{\infty} m^2 \exp(-\pi m^2) = \sum_{m=-\infty}^{\infty} \exp(-\pi m^2)\,. \qquad (65)$$

The latter can be interpreted as an equality connecting $\Theta_3''(0|i)$ and $\Theta_3(0|i)$ where $\Theta_3(z|\tau)$ is the theta function (See Ref. 14, page 471).

V. CONCLUSIONS

The connection established in this paper between wave functions $\langle k,q|f\rangle$ in the kq-representation and amplitudes $\langle \alpha_{mn}|f\rangle$ (or, more generally, $\langle v_{mn}|f\rangle$) of the same state $|f\rangle$ on von Neumann lattices has its origin in the role played by the variables k and q in quantum mechanics. These variables were originally introduced as quantum mechanical representation based on discrete commuting translations in phase space.[20] But it is not hard to see that these translations are exactly the ones that generate a von Neumann lattice. One should therefore anticipate that the kq-representation will be closely related to von Neumann lattices. This is further explained in Appendix B. The variables k and q and two-dimensional vectors on a von Neumann lattice in the phase plane are in some sense conjugate to one another.[16] The formulas in this paper verify this anticipation. The interpretation of the amplitudes $\langle \alpha_{mn}|f\rangle$ as Fourier coefficients of periodic distributions is clearly a consequence of the connection between the variables k and q and von Neumann lattices. As is known, k and q are purely quantum mechanical in their nature and they have no classical analog.[11] Von Neumann lattices are also quantum mechanical structures with a unit cell of exactly the area h. The established formulas in this paper between the wave functions $\langle k,q|f\rangle$ and the amplitudes $\langle \alpha_{mn}|f\rangle$ for a given state $|f\rangle$ can be seen as a formal expression of the physical connection between the variables k and q and von Neumann lattices.

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APPENDIX A

Some properties of the wave function in the kq-representation referred to in the text are given here.

The state in this representation consists of the functions square-integrable on the kq-cell ($0 \le k < 2\pi/a$; $0 \le q < a$) satisfying the boundary conditions (16) and (17). [The scalar product is given by (18)]. The boundary conditions are evidently only meaningful for functions with continuity properties. A function $\langle k,q|f\rangle$ is said to be "continuous" if it is the restriction to the kq-cell, of a function continuous on the extended kq-plane satisfying periodicity conditions (16) and (17). (This definition avoids confusion about discontinuities at the "join" when we regard the kq-cell as a torus: $\langle k,q|f\rangle$ is therefore one branch of a continuous but many-valued function on the torus). We denote the class of continuous functions by $\mathcal{C}$, and emphasize that the boundary conditions are included in the definition of continuity. When coming to classify differentiable functions, we have to note that the periodicity conditions (16) and (17) are not conserved under $\partial/\partial k$, but rather under the operation of $\hat{x}$ in (35). In view of this, and of (35), we shall mean by "differentiation" the operation of $\hat{x}$ or $\hat{p}$. The class $\mathcal{C}^n(\mathcal{C}^0 = \mathcal{C})$ consists of these functions $\langle k,q|f\rangle$ that are the restrictions to the kq-cell of functions on the kq-plane continuously differentiable up to order n. For short: $|f\rangle$ belongs to $\mathcal{C}^n$ if the result of successive operations by $\hat{x}$ and/or $\hat{p}$ up to n times is a state still in $\mathcal{C}$. The important class $\mathfrak{D}$ of functions (Sec. III) characterized by $\Delta x \Delta p < \infty$ lies between $\mathcal{C}^1$ and $\mathcal{C}^2$, because here the second derivatives are required only to be square integrable. Again, $|f\rangle$ is called analytic if it is the restriction of a function analytic in the kq-plane and with periodicity (16) and (17). Evidently all the derivatives of an analytic function are analytic, and furthermore they are the states $|f\rangle$ on which we can expand the exponential in the momentum and position shift operators $\exp(i\bar{p}\hat{x}/\hbar)$ and $\exp(-i\bar{x}\hat{p}/\hbar)$, or in the phase-space displacement operators $D(\alpha)$ of (6). All $|N\rangle$ and $|\alpha\rangle$ are analytic. Finally we note that all classes defined above are dense in the Hilbert space and that each one is contained in $\mathcal{C}$.

We remark that if $|f\rangle$ and $|g\rangle$ both belong to a particular one of the above classes, then $\langle g|k,q\rangle\langle k,q|f\rangle$ will belong to the class of strictly doubly periodic functions that corresponds to it in an obvious way. This is important in the Fourier sum expansions (23), (44), or (54).

We now give an elementary proof of the theorem (Sec. III) that due to the periodicity conditions (16) and (17) any continuous function $\langle k,q|f\rangle$ has a zero in the kq-cell. A topological proof can be found in Ref. 17; the present one has been announced before.[10,16] Thus suppose $|f\rangle \in \mathcal{C}$ and write

$$\langle k,q|f\rangle = |\langle k,q|f\rangle| \exp[i\tau(k,q)]. \tag{A1}$$

Imagine $\langle k,q|f\rangle$ defined on the kq-plane, as we are entitled to do. Since the modulus is strictly doubly periodic, it follows from (16) and (17) that

$$\tau(k+2\pi/a,q) = \tau(k,q) + 2\pi l, \tag{A2}$$

$$\tau(k,q+a) = \tau(k,q) + 2\pi l' + ka, \tag{A3}$$

where l and l' are two fixed integers. Setting $q \to q+a$ in (A2) and using (A3), then setting $k \to k+2\pi/a$ in (A3) and using (A2), one gets two expressions for $\tau(k+2\pi/a, q+a)$ differing additively by 2π. But if the modulus in (A1) vanishes nowhere, both it and the phase $\tau(k,q)$ are continuous (in the usual sense) in the kq-plane. Therefore $\langle k,q|f\rangle$ must vanish somewhere.

Naturally this is the situation for all the classes defined earlier and particularly for $\mathfrak{D}$. But it does not appear to be easy to identify the zeros of $\langle k,q|f\rangle$ in many practical cases. The single zero of $\langle k,q|0\rangle$ at $k=\pi/a, q=a/2$, we know from (25). The $\langle k,q|\alpha\rangle$ have a single zero, obtained by displacement from the $|\alpha\rangle = |0\rangle$ case via (5). We can prove that there is always a zero at $(\pi/a, a/2)$ if the wave function $\psi(x)$ in the x-representation is even. In this case, from (15) we have $\langle -k,-q|f\rangle = \langle k,q|f\rangle$, where the result follows using (16) and (17). Again, if $\psi(x)$ is odd, there are zeros at $(0,0)$, $(\pi/a, 0)$ and $(0, a/2)$. For from (15) $\langle -k,-q|f\rangle = -\langle k,q|f\rangle$, and the result follows by a similar argument.

APPENDIX B

In this Appendix we express the relationship between the kq-representation and the von Neumann lattice in group theoretical terms, and situate the basic Fourier expansion formula in this framework.

It is well known[8,10,11,20] that the set of phase-space translations $(-1)^{mn}D(\alpha_{mn})$ associated with the von Neumann lattice form an infinite discrete abelian group [the factor $(-1)^{mn}$ ensures correct group multiplication]. The unit cell of the von Neumann lattice can be viewed as a Brillouin zone whose points k, q $(0 \le q < a; 0 \le k < 2\pi/a)$ label the irreducible representations of the group. Let us denote the carrier spaces of the irreducible representations, i.e., the simultaneous eigenfunctions of the group translations,[11] by kets $|k,q\rangle$ where by definition

$$(-1)^{mn}D(\alpha_{mn})|k,q\rangle = \exp(i(2\pi/a)qm - iakn)|k,q\rangle. \tag{B1}$$

In the x-representation the $|k,q\rangle$ are distributions of the form[11]

$$\langle x|k,q\rangle = \left(\frac{2\pi}{a}\right)^{1/2} \sum_{s=-\infty}^{\infty} \exp(iksa)\delta(x-q-sa)$$

and they satisfy the orthonormality and closure conditions

$$\langle k,q|k',q'\rangle = \exp[-i(q-q')k]\Delta(q-q')\Delta(k-k'); \qquad \int |k,q\rangle\langle k,q|\,dk\,dq = I, \tag{B2}$$

where Δ is the Dirac δ-function on the kq-cell. Equation (B2) expresses the fact that k,q are good labels for a representation of the wave functions.

The projection operators for the irreducible representations of the group are found from a standard formula of group algebra to be

$$|k,q\rangle\langle k,q| = \frac{1}{2\pi}\sum_{mn}(-1)^{mn}\exp\left(-i\frac{2\pi}{a}qm + iakn\right)D(\alpha_{mn}). \tag{B3}$$

One can see using (8) that the Fourier expansion (44) is just a matrix element of (B3) between states $|v\rangle$ and $|f\rangle$. And this observation gives a precise meaning to the equality in (B3). Equation (B3) can also be used to frame the questions on completeness properties of von Neumann sets in another way. Operate on $|v\rangle$ and use (8)

$$|k,q\rangle\langle k,q|v\rangle = \frac{1}{2\pi}\sum_{mn}(-1)^{mn}\exp\left(-i\frac{2\pi}{a}qm + iakn\right)|v_{mn}\rangle. \tag{B4}$$

Also from (B4)

$$|v_{mn}\rangle = (-1)^{mn}\int |k,q\rangle \exp\left(i\frac{2\pi}{a}qm - iakn\right)\langle k,q|v\rangle\,dk\,dq. \tag{B5}$$

Relations (B4) and (B5) are the transformation and its inverse between the orthonormal (continuous) basis of of kets $|k,q\rangle$ and the discrete von Neumann set $\{|v_{mn}\rangle\}$. The completeness properties of the $|v_{mn}\rangle$ clearly depend on the singularities in this transformation. For example, one can easily see that the transformation is unitary when $|\langle k,q|v\rangle|\equiv 1$, i.e., when the $|v_{mn}\rangle$ form an orthonormal basis. Again, when $\langle k,q|v\rangle$ is smooth and therefore has zeros (Appendix A), the transformation is evidently singular, with consequent overcompleteness problems studied in the text.

In his book,[6] von Neumann posed the question: In view of the noncommutativity of $\hat{x}$ and $\hat{p}$, is it possible to construct "macroscopic" operators $\hat{X}$ and $\hat{P}$ that do commute, but whose spectra are discrete and interpretable as coarsegrained values of position and momentum accurate within $\Delta x \Delta p \approx h$? In our terms can we construct operators $\hat{X}$ and $\hat{P}$ whose eigenvectors form a complete von Neumann set and whose eigenvalues are on the von Neumann lattice

$$\hat{X}|v_{mn}\rangle = na|v_{mn}\rangle; \quad \hat{P}|v_{mn}\rangle = (2\pi\hbar/a)m|v_{mn}\rangle? \tag{B6}$$

If this scheme can be satisfactorily set up, then $\hat{X}$ and $\hat{P}$ would be a pair of operators conjugate to the cyclic variables corresponding to the two generators of the discrete phase-space translation group above, i.e., to

$$\exp i(2\pi/a)\hat{x}; \quad \exp ia\hat{p}/\hbar. \tag{B7}$$

The set of amplitudes $\langle v_{mn}|f\rangle$ of any state $|f\rangle$ on the simultaneous eigenstates of $\hat{X}$ and $\hat{P}$ would provide a discrete quantum mechanical representation, conjugate to the continuous representation $\langle k,q|f\rangle$ of amplitudes on the simultaneous eigenstates $|k,q\rangle$ of (B7) [via (B1)]. Equations (B4) and (B5) transform one representation into the other. Evidently, therefore, the question of the existence of $\hat{X}$ and $\hat{P}$ and the properties of the corresponding representation $\langle v_{mn}|f\rangle$ are directly related to the results of this paper, and notably to the nature of the transformations (B4) and (B5). In the orthonormal case ($|\langle k,q|v\rangle|\equiv 1$), where (B4) and (B5) are unitary, the corresponding $\hat{X}$ and $\hat{P}$ have been constructed.[16] If $\langle k,q|v\rangle\equiv 1$, for example, one finds $\hat{X}=i\partial/\partial k$; $\hat{P}=-i\partial/\partial q$ as may be checked from (8); if $\langle k,q|v\rangle$ is a phase, $\hat{X}$ and $\hat{P}$ are gauged accordingly.[21] The transformations (B4) and (B5) are comparable in this case to the unitary transformations linking the conjugate x- and p-representations

$$|p\rangle = \frac{1}{(2\pi\hbar)^{1/2}}\int_{-\infty}^{\infty}\exp\left(i\frac{px}{\hbar}\right)|x\rangle dx \tag{B8}$$

and its inverse. Here $|x\rangle$ and $|p\rangle$ are respectively the orthonormal eigenfunctions of the conjugate variables $\hat{x}$ and $\hat{p}$. Again here, a phase change in (B8) means a gauge change in the momentum operator.

The nonunitary case for (B4) and (B5) is, as we have seen, more complicated, and the determination of $\hat{X}$ and $\hat{P}$, closely linked with the properties of the von Neumann set $|v_{mn}\rangle$, is not yet satisfactory achieved. This problem can also be compared with a corresponding one for the $\hat{x}$ and $\hat{p}$. The basic relation corresponding to (B3) is

$$|x\rangle\langle x| = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\exp\left(-i\frac{px}{\hbar}\right)\exp\left(i\frac{p\hat{x}}{\hbar}\right)dp. \tag{B9}$$

Operating on arbitrary $|v\rangle$ we obtain a relation that parallels (B4). Then the properties of the transformation are dependent on the nature of the function $v(x)\equiv\langle x|v\rangle$ and the whole investigation can be done in the same way as in this paper, replacing Fourier sums by Fourier integrals. In (B9), the investigation will concern the relationship between the orthonormal basis $\{|x\rangle; -\infty < x < \infty\}$ and the set $\{|v_p\rangle \equiv \exp(ip\hat{x}/\hbar)|v\rangle; -\infty < p < \infty\}$.

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Quantum field theory of singletons. The Rac

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Dirac singletons are the most elementary physical objects on de Sitter space; massless particles are two-singleton states. Singleton field theory is characterized by a gauge structure that is strikingly similar to that of massless particles. The Rac and the Di are described by a scalar field and a spinor field, respectively, so the appearance of a fully developed gauge structure is remarkable. In this paper Rac field theory is quantized by using an indefinite metric, in close analogy with the Gupta–Bleuler method of electrodynamics. A Lagrangian theory of interacting Rac fields is also given, including the unique invariant local-interaction between Racs.

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I. INTRODUCTION

It is axiomatic to elementary particle physics that the objects of greatest interest are the most elementary ones. In a relativistic theory the most elementary objects are associated with unitary, irreducible representations of the space–time group. In Minkowski space this is the Poincaré group, and the UIR's that are widely and justifiably regarded as the most important ones are the representations with zero mass and discrete helicity—the massless ones, for short. In de Sitter space the space–time group is (some covering of) SO(3, 2). This group also has massless representations,[1] quite analogous to those of the Poincaré group, that describe neutrinos,[2] electrodynamics,[2] weak gravitational fields,[3] supergravity, and so on,[4,5] as well as Yang–Mills fields. But these massless UIR's of the de Sitter group are not the most elementary objects, for the set of all two-particle singleton states can be identified with the set of all massless one-particle states.[6]

The singletons are a pair of unitary, irreducible representation of SO(3, 2), first discovered by Dirac,[7] with a remarkably reduced spectrum: these representations remain irreducible when restricted to the Lorentz subgroup. The Rac is spinless and the Di is spin 1/2; both come with either positive or negative energy and there are no others. Here we deal with Racs only.

The Rac can be realized in terms of a scalar field, on a space of solutions of a covariant Klein–Gordon equation

$$(\Box - \tfrac{5}{12}\Lambda)\varphi = 0.$$

Here Λ is the (positive) cosmological constant and the following describes a situation that arises only for the particular choice of the numerical factor shown. One finds three spaces of solutions:

$$\mathscr{D}'_- \supset \mathscr{D}' \supset \mathscr{D}'_g,$$

each of which is invariant for the action of the de Sitter group. This action is nondecomposable; that is, there is no invariant subspace that is complementary to $\mathscr{D}'_g$ in $\mathscr{D}'$ or to $\mathscr{D}'$ in $\mathscr{D}'_-$. The representations realized on $\mathscr{D}'_g$ and on $\mathscr{D}'/\mathscr{D}'_g$ are unitary and the Rac is the latter. This structure is in every respect remarkably close to that of electrodynamics.

The main result of this paper is the construction of a Rac quantum field theory. It is necessary to introduce an indefinite metric and the scheme of quantization is essentially that of Gupta and Bleuler. This work is done directly on de Sitter space and also, as in another paper,[1] on the cone at infinity. Causality is not easily investigated at infinity, and one purpose of this paper is to show that the Rac field is local, so that Rac propagation in de Sitter space is causal. The commutator $[\phi(y), \phi(y')]$ does indeed vanish for spacelike separation. Another purpose is to show that gauge problems and indefinite metric quantization are phenomena that can arise in a scalar field theory. For both of these reasons we believe that it is worthwhile to carry out the more complicated construction of a local field theory on de Sitter space itself. An action principle can also be formulated; it includes a uniquely determined invariant interaction between Racs.

This field theory of Racs is an eminently physical theory; in particular it is unitary and local. One-Rac states are practically impossible to detect,[1,6] for purely kinematical reasons; no special feature of the interaction needs to be arranged to bring this about. Two-Rac states are interpretable as massless particles with even spins. Odd spins and half-integral spins will be included in a theory of Dis and Racs. So far we have an interacting quantum field theory that includes massless particles with all even spins.

It should be stressed that the quantization procedure adopted in this paper is not the only one imaginable. Other types of quantization of the Rac field may turn out to be more appropriate for the applications to massless particles.

II. WAVE EQUATION AND SOLUTIONS

As usual, we embed de Sitter space in $\mathbb{R}^5$ by means of a differentiable and locally invertible map $(x^0, x^1, x^2, x^3) \to (y^0, y^1, y^2, y^3, y^5)$, with $y^2 = \delta^{\alpha\beta} y_\alpha y_\beta = y_0^2 + y_5^2 - \vec{y}^2 = \rho^{-1}$, $\rho > 0$ and fixed. De Sitter space is the universal covering space M of this hyperboloid. When it becomes necessary to use a global coordinate system for M we shall employ the following: $(t, \vec{y}) = (t, y_1, y_2, y_3)$, with each coordinate running independently over $\mathbb{R}$,

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$$y_0 = Y \sin t, \quad y_5 = Y \cos t, \tag{2.1}$$
$$Y = +(y_0^2 + y_5^2)^{1/2} = (\rho^{-1} + r^2)^{1/2}, \quad r^2 = \vec{y}^2.$$

The generators of infinitesimal space–time transformations act on differential functions on M by

$$L_{\alpha\beta} = i(y_\alpha \partial_\beta - y_\beta \partial_\alpha), \tag{2.2}$$
$$\partial_\alpha = \partial / \partial y^\alpha, \quad \alpha, \beta = 0, 1, 2, 3, 5.$$

Consider a (classical) scalar field φ on M, satisfying the wave equation[2]

$$[(1/2) L_{\alpha\beta} L^{\alpha\beta} - E_0(E_0 - 3)]\varphi = 0,$$

or

$$[y^2 \partial^2 - \hat{N}(\hat{N} + 3) + E_0(E_0 - 3)]\varphi(y) = 0, \tag{2.3}$$
$$\partial^2 = \delta^{\alpha\beta} \partial_\alpha \partial_\beta, \quad \hat{N} = y^\alpha \partial_\alpha.$$

The real parameter E_0 plays a role similar to that of mass in Minkowski space.[2] The following functions are solutions of Eq. (2.3)[8]:

$$\varphi_{KLM}(y) = \frac{1}{(L+\frac{1}{2})!} \left[\frac{(L+K+E_0-1)!(L+K+\frac{1}{2})!}{K!(K+E_0-\frac{3}{2})!} \right]^{1/2} \times \rho^{(1/2)(1/2 - E_0 - 2K)} e^{-iEt} Y^{-E} r^L Y_{LM}(\hat{y}) \times {}_2F_1(-K, -E_0 - K + \tfrac{3}{2}; L + \tfrac{3}{2}; -\rho r^2), \tag{2.4}$$
$$M = -L, -L+1, \ldots, L, \quad L = 0, 1, \cdots,$$
$$K = 0, 1, \cdots, \quad E = E_0 + L + 2K.$$

Each of these functions is an eigenfunction of the time translation operator $L_{05} = i\,\partial/\partial t$ with eigenvalue E. The functions $Y_{LM}(\hat{y})$, $\hat{y} = \vec{y}/r$, are spherical harmonics.

When $E_0 > \frac{1}{2}$, then this set is a complete set of positive energy solutions of Eq. (2.3), orthonormal with respect to the inner product

$$(\varphi, \varphi') = \int_{\mathbb{R}^3} \overline{\varphi(t, \vec{y})}\, i \overleftrightarrow{\partial_t} \varphi(t, \vec{y}) d^3y / Y^2. \tag{2.5}$$

Let $\mathscr{D}$ be the space of finite linear combinations of the functions (2.4), completable to the Hilbert space $L^2(\mathbb{R}^3, d^3y/Y^2)$. The action (2.2) on $\mathscr{D}$ is integrable to a unitary irreducible representation of SO(3, 2) on L^2 that we denote $D(E_0, 0)$.[2]

The representation Rac $= D(\frac{1}{2}, 0)$ is the limit of $D(E_0, 0)$ as $E_0 \to \frac{1}{2}$ from above in very much the same sense that the massless representations of the Poincaré group are limits of the massive ones. Note, however, that the Rac is *not* a "massless" representation of SO(3, 2). When $E_0 \to \frac{1}{2}$, then $\lim (E_0 - \frac{1}{2})^{-1/2} \varphi_{0LM}$ and $\lim \varphi_{KLM}$, $K \geqslant 1$, exist. The representation defined by (2.2) now becomes nondecomposable. The span of $\lim \varphi_{KLM}$, $K \geqslant 1$, is invariant and carries the UIR $D(\frac{5}{2}, 0)$. The Rac is induced on the quotient space. In a close analogy with electrodynamics, the Rac states correspond to the transverse photons and the invariant subspace corresponds to the longitudinal photons. To quantize electrodynamics one needs to introduce scalar photons as well, and the situation is not different here.

Equation (2.3) is unchanged when E_0 is replaced by $3 - E_0$, but (2.4) is not, and this observation leads to a second set of solutions. It is convenient to define K such that its range is 1, 2, ⋯ for this new set, and to introduce $\epsilon = E_0 - \frac{1}{2}$ instead of E_0; then one gets

$$\varphi'_{KLM} = \frac{1}{(L+\frac{1}{2})!} \left[\frac{(L+K+\frac{1}{2}-\epsilon)!(L+K-\frac{1}{2})!}{(K-\epsilon)!(K-1)!} \right]^{1/2} \rho^{(\epsilon - 2K)/2} \times e^{-iEt} Y^{-E} r^L Y_{LM}(\hat{y}) \times {}_2F_1(-K+\epsilon, 1-K; L+\tfrac{3}{2}; -\rho r^2), \tag{2.6}$$
$$M = -L, -L+1, \ldots, L, \quad L = 0, 1, \ldots,$$
$$K = 1, 2 \cdots, \quad E = \tfrac{1}{2} - \epsilon + L + 2K.$$

When $\epsilon < 2$, $E_0 < \frac{5}{2}$ or $3 - E_0 > \frac{1}{2}$), then this set is another complete set of positive energy solutions of Eq. (2.3), orthonormal with respect to (2.5). Let $\mathscr{D}'$ be the space of finite linear combinations of the functions (2.6); the action (2.2) on $\mathscr{D}'$ is integrable to $D(3 - E_0, 0)$. As $E_0 \to \frac{1}{2}$ all the functions (2.6) remain finite and normalized and $D(3 - E_0, 0) \to D(\frac{5}{2}, 0)$. It will be seen that these states correspond to the scalar photons of electrodynamics. We are now ready to examine the limit $E_0 \to \frac{1}{2}$ in greater detail.

With $\epsilon = E_0 - \frac{1}{2}$, we copy (2.4)

$$\varphi_{KLM} = \frac{1}{(L+\frac{1}{2})!} \left[\frac{(L+K+\frac{1}{2})!(L+K-\frac{1}{2}+\epsilon)!}{K!(K-1+\epsilon)!} \right]^{1/2} \rho^{(-\epsilon - 2K)/2} \times e^{-iEt} Y^{-E} r^L Y_{LM}(\hat{y}) \times {}_2F_1(-K, 1-K-\epsilon; L+\tfrac{3}{2}; -\rho r^2),$$
$$K = 0, 1, \cdots, \quad E = \tfrac{1}{2} + \epsilon + L + 2K.$$

When $\epsilon \to 0$ the following linear combinations remain finite ($K = 1, 2, \cdots; E = \frac{1}{2} + L + 2K$):

$$\varphi_{KLM} \to \frac{1}{(L+\frac{1}{2})!} \left[\frac{(L+K+\frac{1}{2})!(L+K-\frac{1}{2})!}{K!(K-1)!} \right]^{1/2} \rho^{-K} \times e^{-iEt} Y^{-E} r^L Y_{LM}(\hat{y}) \times {}_2F_1(-K, 1-K; L+\tfrac{3}{2}; -\rho r^2), \tag{2.7}$$

$$\varphi_{LM} = \epsilon^{-1/2} \varphi_{0LM} \to (L+\tfrac{1}{2})^{-1/2} e^{-it(L+1/2)} Y^{-L-1/2} r^L Y_{LM}(\hat{y}), \tag{2.8}$$

$$\varphi_{\bar{K}LM} = \epsilon^{-1}(\varphi_{KLM} - \varphi'_{KLM}). \tag{2.9}$$

The functions φ_{KLM} and φ_{LM} are one-valued on the double covering of the hyperboloid, but $\varphi_{\bar{K}LM}$ are defined on the universal covering only. After passage to the limit $\epsilon \to 0$, let $\mathscr{V}_-$ denote the set of finite linear combinations of all these basis vectors, let $\mathscr{V}$ be the subspace spanned by φ_{LM} and φ_{KLM}, and let $\mathscr{V}_g$ be the span of φ_{KLM}:

$$\mathscr{V}_g = \operatorname{Span}\{\varphi_{KLM}\} \subset \mathscr{V},$$
$$\mathscr{V} = \operatorname{Span}\{\varphi_{KLM}, \varphi_{LM}\} \subset \mathscr{V}_-,$$
$$\mathscr{V}_- = \operatorname{Span}\{\varphi_{KLM}, \varphi_{LM}, \varphi_{\bar{K}LM}\}.$$

For the action of SO(3, 2) defined by (2.2), $\mathscr{V}_g$ is an invariant subspace of $\mathscr{V}$ and $\mathscr{V}$ is an invariant subspace of $\mathscr{V}_-$. There is no invariant complement in either case and the representations that are induced in $\mathscr{V}_-$ and in $\mathscr{V}$ are nondecomposable.[9] The space $\mathscr{V}_g$ is completable[2] to the Hilbert space $L^2(\mathbb{R}^3, d^3y/Y^2)$. The Rac is the UIR realized in a Hilbert space that is easily constructed as an l^2 space by completion of $\mathscr{V}/\mathscr{V}_g$.

III. COVARIANT PROPAGATOR

For $2 > \epsilon > 0$ one finds[10]

$$\sum_{KLM} \varphi_{KLM}(y)\, \overline{\varphi_{KLM}(y')} = K(Z)$$
$$= \frac{\rho^{1/2}}{4\pi} \frac{(\epsilon - \frac{1}{2})!}{(\frac{1}{2})!(\epsilon - 1)!} \zeta^{1/2+\epsilon} {}_2F_1(\tfrac{3}{2}, \tfrac{1}{2} + \epsilon; \epsilon; \zeta^2), \quad (3.1)$$

$$\sum_{KLM} \varphi'_{KLM}(y)\, \overline{\varphi'_{KLM}(y')} = K'(Z)$$
$$= \frac{\rho^{1/2}}{4\pi} \frac{(\frac{3}{2} - \epsilon)!}{(\frac{1}{2})!(1 - \epsilon)!} \zeta^{5/2-\epsilon} {}_2F_1(\tfrac{3}{2}, \tfrac{5}{2} - \epsilon; 2 - \epsilon; \zeta^2), \quad (3.2)$$
$$\zeta = Z - (Z^2 - 1)^{1/2},$$
$$Z = \rho y \cdot y'.$$

The separation between y and y' is spacelike if $|Z| > 1$, timelike if $|Z| < 1$. If $Z > 1$, then $(Z^2 - 1)^{1/2} > 0$; if in addition $|t - t'| < \pi$, then also $\zeta^{5/2-\epsilon} > 0$. If y and y' are relatively timelike, then $(Z^2 - 1)^{1/2} = i|1 - Z^2|^{1/2}\epsilon(y, y')$, where $\epsilon(y, y') = +1(-1)$ when y is in the future (past) of y'.[11] The functions K and K' are defined as analytic functions of Z in a complex plane cut along the real axis from $-\infty$ to $+1$. The sums (3.1) and (3.2) converge for real y, y' if $Z > 1$.[12]

The idea is to construct a local field theory in which the field commutator is the discontinuity of a function such as these, so that the fields will commute at spacelike separation. The problem is to pass to the limit $\epsilon \to 0$ in (3.1) without loosing the contribution of the Rac states to the sum.

Let us write (3.1), after multiplication by ϵ^{-1}, so as to exhibit what happens as $\epsilon \to 0$. Using the definition (2.8), we get

$$\sum_{LM} \varphi_{LM}(y)\, \overline{\varphi_{LM}(y')} + \epsilon^{-1} \sum_{\substack{KLM \\ K \neq 0}} \varphi_{KLM}(y)\, \overline{\varphi_{KLM}(y')}$$
$$= \epsilon^{-1} K(Z)$$
$$= \frac{\rho^{1/2}}{4\pi} \frac{(\epsilon - \frac{1}{2})!}{(\frac{1}{2})!\epsilon!} \zeta^{1/2+\epsilon} \left[1 + \epsilon^{-1} \sum_{n=1}^{\infty} \frac{(\frac{3}{2})_n (\frac{1}{2} + \epsilon)_n}{n!(\epsilon)_n} \zeta^{2n} \right].$$

Both sides contain terms of order ϵ^{-1}, but there is no invariant way to separate out a finite part. In fact, the first sum, which in a sense is the Rac contribution, is not an invariant function. This is, of course, due to the fact that there is no invariant complement to $\mathscr{V}_g$ in $\mathscr{V}$.

In order to obtain a meaningful result we must include the φ''s. Consider

$$\epsilon^{-1}[K(Z) - K'(Z)]$$
$$= \sum_{LM} \varphi_{LM}\, \overline{\varphi_{LM}} + \epsilon^{-1} \sum_I (\varphi_I\, \overline{\varphi_I} - \varphi'_I\, \overline{\varphi'_I}), \quad (3.3)$$

where I stands for KLM and the indefinite metric is already apparent. Introducing $\varphi_{\bar{K}LM}$, as defined by (2.8), one gets

$$= \sum_{LM} \varphi_{LM}\, \overline{\varphi_{LM}} + \mathrm{Re}\left[\sum_I \varphi_{\bar{I}} (\overline{\varphi_I} + \overline{\varphi'_I}) \right]. \quad (3.4)$$

In this expression each term remains finite as $\epsilon \to 0$. Of course, one could add any finite multiple of K'.

The function K is a Gegenbauer function of the second kind:[13]

$$K(Z) = (\rho^{1/2}/4\pi^2)(Z^2 - 1)^{-1/2} e^{-i\pi} Q^{1}_{\epsilon - 3/2}(Z), \quad (3.5)$$

and[14]

$$\epsilon^{-1}[K(Z) - K'(Z)] = \frac{\rho^{1/2}}{4} \frac{\tan \pi\epsilon}{\pi\epsilon} (Z^2 - 1)^{-1/2} \times P^{1}_{\epsilon - 3/2}(Z). \quad (3.6)$$

This has the following limit as $\epsilon \to 0$:[15]

$$K_{\mathrm{Rac}}(Z) = (\rho^{1/2}/4)(Z^2 - 1)^{-1/2} P^{1}_{1/2}(Z)$$
$$= 2^{-3/2} \rho^{1/2} \pi^{-1} \Big\{ Z^{-1/2} - \tfrac{3}{8} Z^{-5/2} \sum_{n=0}^{\infty} \frac{(\frac{5}{4})_n (\frac{7}{4})_n}{n!(n+1)!}$$
$$\times [\ln(2Z) + \psi(n) + \psi(n+1) - 2\psi(3/2 + 2n)] \Big\}. \quad (3.7)$$

Another expression is

$$K_{\mathrm{Rac}}(Z) = (\rho^{1/2}/2\pi) \Big\{ \zeta^{1/2} + \tfrac{3}{45} \zeta^{5/2} \sum_{n=0}^{\infty} \frac{(\frac{3}{2})_n (\frac{5}{2})_n}{n!(n+1)!} \zeta^{2n}$$
$$\times [\ln \zeta^2 - h_n + \mathrm{const}] \Big\}. \quad (3.8)$$

In these formulas ψ is the logarithmic derivative of the Γ function and h_n is a combination of ψ functions with different arguments. If one adds a finite multiple of $K'(Z)$, it merely affects the value of the constant.

The function K_{Rac} is defined in the complex Z plane, cut from $-\infty$ to $+1$. It thus preserves those properties of K and K' that are necessary in a local field theory. The causal structure of de Sitter space and of the cone is reviewed in the Appendix.

IV. FREE FIELD QUANTIZATION

The functions $\varphi_{KLM}, \varphi_{LM}, \varphi_{\bar{K}LM}$ introduced by (2.6)–(2.8) have finite limits as $\epsilon \to 0$. From now on we use these same symbols to denote the functions obtained by passage to the limit. We shall introduce a set of creation and destruction operators a_{KLM}, b_{LM}, c_{KLM} and their adjoints, with commutation relations to be given shortly, and we shall define the free quantized field operator by

$$\varphi(y) = \sum_I \varphi_I(y) a_I + \sum_{LM} \varphi_{LM}(y) b_{LM}$$
$$+ \sum_I \varphi_{\bar{I}}(y) c_I + \mathrm{h.c.} \quad (4.1)$$

Having determined the propagator,

$$K_{\mathrm{Rac}}(Z) = \sum_{LM} \varphi_{LM}(y)\, \overline{\varphi_{LM}(y')}$$
$$+ \sum_I \left[\varphi_{\bar{I}}(y)\, \overline{\varphi_I(y')} + \varphi_I(y)\, \overline{\varphi_{\bar{I}}(y')} \right], \quad (4.2)$$

we shall choose commutation relations for the creation and distruction operators that will ensure that

$$[\varphi(y), \varphi(y')] = K^{+}_{\mathrm{Rac}}(Z) - K^{-}_{\mathrm{Rac}}(Z), \quad (4.3)$$

where $K^{+}_{\mathrm{Rac}}(Z)$ is the boundary values of the analytic function K_{Rac}, from above if $\sin(t - t') > 0$.[12]

To ensure the validity of (4.3) we shall postulate the following commutation relations:

$$[b_{LM}, b^*_{L'M'}] = \delta_{LL'}\delta_{MM'},$$
$$[a_I, c^*_{I'}] = [c_I, a^*_{I'}] = \delta_{II'}. \quad (4.4)$$

Other commutators vanish. A Fock space with indefinite metric is constructed by postulating a cyclic vector $|0\rangle$ with the property that

$$a_I|0\rangle = b_{LM}|0\rangle = c_I|0\rangle = 0. \quad (4.5)$$

A "physical subspace" may be defined as the subspace of all states with the property

$$c_I\psi = 0. \quad (4.6)$$

This is analogous to the Lorentz condition $\partial\cdot A^+\psi = 0$ in quantum electrodynamics. This space contains quanta associated with the subspace $\mathscr{V}$ introduced in Sec. II, and has a positive semidefinite metric. The subspace of zero-norm states consists of all states with at least one a-excitation; these quanta are associated with $\mathscr{V}_g$. The actual physical multi-Rac states are in the completion of the quotient of the "physical subspace" by this zero-norm subspace.

The simplest way to pass to the quotient space is to replace the fields by their limits at spatial infinity. We prefer to extrapolate from (the double covering of) the de Sitter hyperboloid, to $y^2 > 0$, by fixing the degree of homogeneity to be $-1/2$, and then passing to the limit $y^2 = 0$, with $\vec{y}$, t fixed. This limit is the same as the limit at spatial infinity, in the sense that

$$r^{1/2}\lim_{y^2\to 0}\phi(y) = \lim_{r\to\infty} r^{1/2}\phi(y).$$

In this limit all the gauge fields vanish. From now on we suppose that this has been done, and we shall henceforth use the letters u, v to denote Rac coordinates on the cone. Here is a summary of the conventions used:

$$u^2 = u_0^2 + u_5^2 - \vec{u}^2 = 0, \quad u_0 = U\sin t,\ u_5 = U\cos t, \quad (4.7)$$
$$U = (u_0^2 + u_5^2)^{1/2} = |\vec{u}|, \quad \hat{u} = \vec{u}/U, \quad (4.8)$$
$$L_{\alpha\beta}\phi(u) = i(u_\alpha\partial_\beta - u_\beta\partial_\alpha)\phi(u), \quad (4.9)$$
$$\phi(u) = U^{1/2}\boldsymbol{\phi}(t, \hat{u}). \quad (4.10)$$

Instead of the wave equation (2.3) we have

$$\partial^2\phi(u) = 0, \quad (u\cdot\partial_u + \tfrac{1}{2})\phi(u) = 0, \quad (4.11)$$

or

$$(\partial_t^2 + \vec{L}^2 + \tfrac{1}{4})\boldsymbol{\phi}(t, \hat{u}) = 0, \quad \vec{L}^2 = \tfrac{1}{2}\sum(L_{ij})^2. \quad (4.12)$$

This can be obtained by variation of the invariant action

$$A = \int_{S_1\times S_2} dt\, d\hat{u}\tfrac{1}{2}[\boldsymbol{\phi}_t^2 - \boldsymbol{\phi}_\theta^2 - (1/\sin^2\theta)\boldsymbol{\phi}_\varphi^2 - \tfrac{1}{4}\boldsymbol{\phi}^2]. \quad (4.13)$$

Here $\boldsymbol{\phi}_t = \partial\boldsymbol{\phi}/\partial t$, etc. The invariant, indefinite inner product, canonically associated with this action, is

$$(\boldsymbol{\phi}, \boldsymbol{\phi}') = \int_{S_2} \bar{\boldsymbol{\phi}}\, i\overleftrightarrow{\partial}_t\boldsymbol{\phi}\, d\hat{u}. \quad (4.14)$$

The positive energy, stationary solutions of (4.12) [compare (2.8)],

$$\boldsymbol{\phi}_{LM}(t, \hat{u}) = (2L+1)^{-1/2}e^{-it(L+1/2)}Y_{LM}(\hat{u}) = U^{1/2}\phi_{LM}(u), \quad (4.15)$$

are orthonormal with respect to (4.14). We are now ready to define the free Rac quantized field. To do this on de Sitter space required dealing with gauge problems and indefinite metric. On $S_1\times S_2$ we have no gauge problems, since all gauge fields vanish there.

The most straightforward quantization procedure, and the one we shall adopt in this paper, consists of introducing creation and destruction operators associated with the solutions (4.15), with conventional Bose–Einstein commutation relations:

$$[b_I, b_{I'}^*] = \delta_{II'}, \quad I = (L, M), \quad (4.16)$$

the other commutators vanishing. The free quantized field

$$\phi(u) = \sum_I \phi_I(u)b_I + \overline{\phi_I(u)}\, b_I^*), \quad (4.17)$$

is thus a Hermitean Bose field, acting on the standard Fock space that is constructed in a unique vacuum state $|0\rangle$, satisfying $b_I|0\rangle = 0$.

The two-point Wightman function is

$$\langle 0|\phi(u)\phi(v)|0\rangle = \sum_I \phi_I(u)\overline{\phi_I(v)} \equiv D(u, v). \quad (4.18)$$

After multiplying this by $(UV)^{1/2}$ one obtains the distribution

$$\mathbf{D}(t, \hat{u}; t', \hat{v}) = \frac{1}{4\pi}\sum_L e^{-i\tau(L+1/2)}P_L(\hat{u}\cdot\hat{v}) \quad (4.19)$$
$$= \frac{1}{4\pi}(2\cos\tau - 2\hat{u}\cdot\hat{v})^{-1/2}. \quad (4.20)$$

The last formula is valid in the following sense: the distribution $\mathbf{D}$ is the limit of the analytic function (4.20) as $\tau = t - t'$ tends to the real axis from below.

Distributions $\mathbf{D}^\pm$ will now be defined by

$$\mathbf{D}^\pm(t, \hat{u}; t', \hat{v}) = (1/4\pi)(2\cos\tau \pm i\epsilon - 2\hat{u}\cdot\hat{v})^{-1/2}. \quad (4.21)$$

These are boundary values of an analytic function of $\cos\tau$, defined in the complex plane cut from $-\infty$ to $\hat{u}\cdot\hat{v}$. We shall always interpret $\mathbf{D}$ and $\mathbf{D}^\pm$ in this way, and permit ourselves the abusive notations

$$D(u, v) = (1/4\pi)(2u\cdot v)^{-1/2} \quad (4.22)$$
$$D^\pm(u, v) = (1/4\pi)(2u\cdot v \pm i\epsilon)^{-1/2}. \quad (4.23)$$

The commutator

$$[\phi(u), \phi(v)] = \epsilon(\sin\tau)(D^+ - D^-), \quad (4.24)$$

vanishes when $\cos\tau > \hat{u}\cdot\hat{v}$; that is, when the separation between u and v is spacelike-even. (The causal structure of de Sitter space and of the cone are reviewed in the Appendix.) The equal time commutator $[\boldsymbol{\phi}(t, \hat{u}), \boldsymbol{\phi}(t, \hat{v})]$ vanishes, and

$$\left[\boldsymbol{\phi}(t, \hat{u}), \frac{d}{dt}\boldsymbol{\phi}(t, \hat{v})\right] = i\sum_I Y_{LM}(\hat{u})\overline{Y_{LM}(\hat{v})}$$
$$= i\delta^2(\hat{u}, \hat{v}), \quad (4.25)$$

where δ^2 is the Dirac δ-function relative to the measure $d\hat{u}$ on S_2. For $|t - t'| < \pi$,

$$T\phi(u)\phi(v) = \begin{cases}\phi(u)\phi(v), & t > t',\\ \phi(v)\phi(u), & t' > t.\end{cases} \quad (4.26)$$

For the vacuum expectation value we have

$$\langle 0|T\phi(u)\phi(v)|0\rangle = -iD_F(u, v) = D^+(u, v), \quad (4.27)$$

$$\mathbf{D}_F(u,v) = \frac{i}{4\pi}\sum_L e^{-i|\tau|(L+1/2)}P_L(\hat{u}\cdot\hat{v}) \tag{4.28}$$

The only SO(3, 2)-invariant interaction between the Racs, of the usual local, polynomial type, that can be added to the action (4.13), is $g_1\phi^6$. Interactions between Racs are therefore characterized by a unique, real coupling constant. [Locally, one can pass to another three-dimensional formulation by projecting the cone on a flat 2 + 1 dimensional Minkowski space; then SO(3, 2) becomes the conformal group of this space. The conformal degree of the Rac is $-1/2$ and $g_1\phi^6$ is the only conformally invariant interaction.] In the next section we shall formulate this theory directly on de Sitter space.

V. LAGRANGIAN FIELD THEORY WITH INTERACTIONS

Instead of extending the fields to $\mathbb{R}^5$, $y^2>0$, and passing to the limit $y^2\to 0$, one may remain on de Sitter space and consider the limit $r\to\infty$ with t, $\hat{y}$ fixed. In this limit

$$\lim r^{1/2}\varphi_{LM}(y) = (L+\tfrac{1}{2})^{-1/2}e^{-it(L+1/2)}Y_{LM}(\hat{y}), \tag{5.1}$$

$$\lim r^{1/2}\varphi_{KLM} = \lim r^{1/2}\varphi_{KLM} = 0,\quad K\geqslant 1.$$

Thus all gauge fields fall off faster than $r^{-1/2}$ as $r\to\infty$. Let a Lagrangian density on de Sitter space be given by $(\hat{N}=y^\alpha\partial_\alpha)$:

$$\begin{aligned}-\mathscr{L} &= \tfrac{1}{4}(L_{\alpha\beta}\varphi)(L^{\alpha\beta}\varphi)+\tfrac{5}{8}\varphi^2+g_1\varphi^6\\ &= -(1/2\rho)(\partial_\alpha\varphi)^2-(\hat{N}\varphi)^2+\tfrac{5}{8}\varphi^2+g_1\varphi^6.\end{aligned} \tag{5.2}$$

If the action is defined by integrating over de Sitter space with an SO(3, 2)-invariant measure then the variational equation is

$$(\tfrac{1}{2}L_{\alpha\beta}L^{\alpha\beta}+\tfrac{5}{4})\varphi+6g_1\varphi^5=0. \tag{5.3}$$

Since the physically important part of the field is periodic, integrating over the universal covering of the hyperboloid is questionable, but if the integration is restricted to the double covering then the gauge fields will give nonvanishing boundary contributions.

The problem is to find an action that is gauge-invariant. Since gauge fields fill off faster at spatial infinity than the physical fields, this can be solved by choosing an action that can be expressed as a surface integral at spatial infinity. In other words, take the action

$$A = 2\int_{-2\pi}^{2\pi}dt\int_{S_2}d\Omega\,\lim_{r\to\infty} r^3\mathscr{L}(t,y,r). \tag{5.4}$$

The function $\mathscr{L}$ is the same as in (5.2); it was constructed so that only physical fields contribute to the limit. Next

$$\begin{aligned}A &= 2\int dt\,d\Omega\int_0^\infty dr\frac{\partial}{\partial r}(r^3\mathscr{L})\\ &= 2\int dt\,d\Omega\int r^2dr(3+r\partial_r)\mathscr{L},\end{aligned}$$

and finally

$$A=\int dy\vec{\partial}\cdot\vec{y}\mathscr{L},$$

$$dy=\delta(y^2-\rho^{-1})d^5y=2dt\ d^3\vec{y}. \tag{5.5}$$

The integral extends over the double covering of the hyperboloid; since the action is gauge-invariant no surface terms at $t=\pm 2\pi$ appear when one integrates by parts. The action (5.5) gives rise to the completely gauge-invariant equation

$$\lim_{r\to\infty} r^3\left|(\tfrac{1}{2}L_{\alpha\beta}L^{\alpha\beta}+\tfrac{5}{4})\varphi+6g_1\varphi^5\right|=0.$$

Wishing to formulate a theory of fields that propagate on de Sitter space we introduce "gauge fixing." Relaxing the invariance requirement for the free Lagrangian we take

$$A=\int dy\mathscr{L}_0+\int dy(3+\hat{N})\mathscr{L}_I,$$

where $\mathscr{L}_0$ is the free Lagrangian and $\mathscr{L}_I$ the interaction. Now we get

$$(\tfrac{1}{2}L_{\alpha\beta}L^{\alpha\beta}+\tfrac{5}{4})\varphi=g_1\varphi^5\delta(\sigma_\infty),$$

where by $\delta(\sigma_\infty)$ we indicate a δ-distribution supported on the surface $S_1\times S_2$ at spatial infinity. In a future paper we hope to develop this theory in greater detail, and to complete its interpretation in terms of massless particles and fields.[16]

APPENDIX

The causal structure on de Sitter space was first described by Castell.[17] The separation between y and y' is said to be spacelike if $|y\cdot y'|>\rho^{-1}$, spacelike-even if $y\cdot y'>\rho^{-1}$ spacelike-odd if $y\cdot y'<-\rho^{-1}$, and timelike if $|y\cdot y'|<\rho^{-1}$. The hyperboloid contains two disconnected regions that are spacelike relative to y', one whose border contains the point y' (this is spacelike-even relative to y') and one whose border contains the point $-y'$ (spacelike-odd relative to y'). There are also two disconnected regions that are timelike relative to y', their borders intersect at y' and at $-y'$. They are distinguished by the sign of $t-t'$, and this is the basis for the invariant definition of the future and the past relative to the

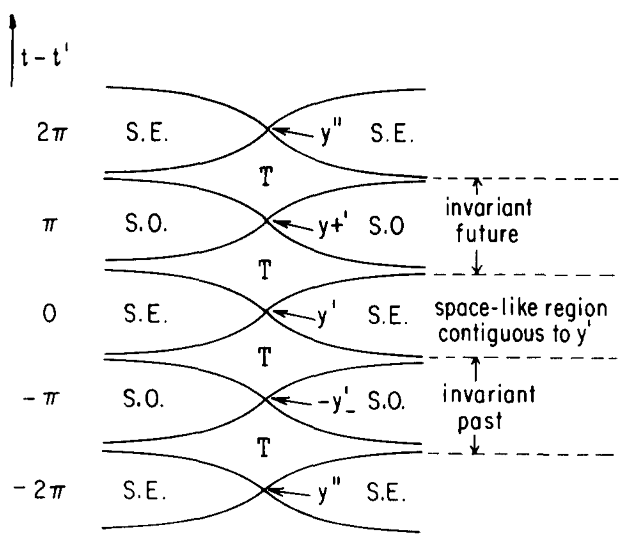

FIG. 1. Double covering of the hyperboloid. The two points marked y'' are identified with each other. The field commutator $[\phi(y),\phi(y')]$ vanishes if y lies in a region marked S(pacelike) E(ven). The regions in which y is timelike relative to y' are marked T(imelike). As one passes to the cone, these regions shrink away, and the past and future are made up of the spacelike-odd regions (marked S.O.) and their boundaries.

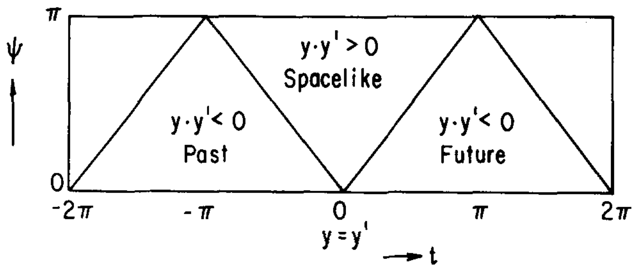

FIG. 2. Double covering of $S_1 \times S_2$, with S_2 represented as a horizontal line.

point y'. The precise definition depends on which covering space is being considered.[8] In the case of the double covering we have two disconnected regions that are spacelike-even relative to y'. We call the future of y' the set of all points y such that $t - t' > 0$ and such that y is not spacelike-even relative to y'; we call the past of y' the set of all points y such that $t - t' < 0$ and such that y is not spacelike-even relative to y'. Figure 1 gives a rough illustration.

In the limit $y^2 \to 0$ this causal structure on the double hyperboloid turns into a causal structure on the double cone. The timelike regions marked T in Fig. 2 shrink away and the past and the future are made up of the limits of the spacelike-odd regions. In order to explain why it is that spacelike-odd regions on the hyperboloid must be considered as lying in the past or in the future, let us consider the propagator-function. The propagator for $D(E_0, 0)$ is given by the boundary values of a function of $Z = \rho y \cdot y'$, cut from $-\infty$ to $+1$. The spacelike-even/timelike/spacelike-odd regions are $Z > 1$, $|Z| < 1$, $Z < -1$, respectively. If E_0 is an integer (as it is for integer spin massless particles), then the cut extends from $Z = -1$ to $Z = +1$ only. (In the case of massless particles it disappears altogether, leaving only poles at $Z = \pm 1$.) In all other cases, including the Rac $= D(\frac{1}{2}, 0)$, the cut extends all the way to $-\infty$. Therefore, if y is spacelike-odd relative to y', then the field operators $\phi(y)$ and $\phi(y')$ do not commute with each other. In the limit $y^2 \to 0$, the cut extends from $-\infty$ to 0 in the variable $y \cdot y'$ except when (as in the case of massless particles) it reduces to a pole.

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Quasicontinual approach to a field theory on a lattice: General theory

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A general theory is systematically presented for handling sets of discrete quantities like values of a field on a lattice, with use of special functions of continuous variables. Those functions, which interpolate their discrete lattice values, form a so-called quasicontinuum. The multiplication rule for interpolating functions, corresponding to the multiplication of lattice sites values of those functions, turns out to be a nonlocal operation. Moreover, the Leibnitz rule for differentiation of a product is invalid here and its defect is found explicitly. The derivatives of interpolating functions at lattice sites may be readily calculated and yield results found earlier by the SLAC (Stanford Linear Accelerator Centre) group.

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I. INTRODUCTION

A new trend in quantum field theory started with the Wilson formulation of gauge theories on a lattice.[1] Instead of writing about the motivations and hopes inspiring this kind of research, we shall be concerned here with some of its problems. In particular, we would like to clarify its mathematical foundations by linking it with similar schemes developed earlier in the theory of elastic media and in the theory of communication.

Indeed, assuming a simple cubic spatial lattice in the Euclidean space R^3 one is dealing with the set of values—let us say a scalar field $\Phi(t,\mathbf{x})$ at lattice sites, $\mathbf{x} = a\mathbf{n}$, where a is the lattice constant and $\mathbf{n} = (n^1,n^2,n^3)$, n^k integers. Immediately the question arises of values of partial derivatives of the field at those points, and a lot of ingenuity, and work, was invested before a satisfactory derivative was defined.[2-4]

Clearly, the problem of finding derivatives $\partial_k \Phi(t,a\mathbf{n})$ would be solved instantly if the field $\Phi(t,\mathbf{x})$ could be restored from its values at the lattice sites. This is not at all a hopeless task if one takes into consideration that the Fourier transform $\tilde{\Phi}(t,\mathbf{p})$ of the field has support confined to the bounded region
$\mathfrak{A} = \{p; -\Lambda \leqslant p_k \leqslant \Lambda, k = 1,2,3; \Lambda = \pi/a\}$.
Hence the field $\Phi(t,\mathbf{x})$, it turns out, admits an analytic continuation, in all its spatial variables, as an entire analytic function. This, together with some technical assumptions, leads to a unique restoration of the field from its values at lattice sites! The partial derivatives of the field coincide with those found by the SLAC group.[4]

Therefore, when dealing with a field theory on a lattice, we find it natural and useful to consider its interpolation—a field having given values at lattice sites. Such a field permits us to use well-developed techniques of continuous analysis for handling discrete quantities. There is, of course, some price to be paid for this convenience, as we will see later.

The interpolation problem is an old one. It starts with the Lagrange formula for an entire analytic function assuming given values at some infinite set of points.[5] In more modern literature it appeared in the theory of communication as the problem of passing information about a continuous function by transmitting through a communication channel only its values at discrete points. A corresponding theorem on reconstruction of a function from its discrete samplings was rediscovered by Kotelnikov and by Shannon.[6] Recently, similar questions were discussed in a theory of elastic media. The so-called quasicontinual approach to crystals, or, more generally, to media with a discrete microstructure was proposed in Refs. 7–9.

We shall describe in the next section the main points of reconstruction of an interpolating field from its values at lattice sites, for the completeness of the paper, and to establish the notation. We borrow freely from Refs. 6, 7, and 9–11. The third, fourth, and partly the fifth sections contain our original results on the multiplication law of interpolating fields and corresponding formfactors. It turns out that a product of two or more fields is a nonlocal operation, and that that Leibnitz rule for differentiation of a product is inapplicable. The formfactors of lower order are found explicitly, and the defect of the Leibnitz rule is calculated. Hence, the price one has to pay for the comfort of using previous methods of continual analysis, when dealing with a field theory on a lattice, is the nonlocality of the corresponding theory, and inapplicability of the Leibnitz rule for differentiation of the specially defined product of two interpolating fields. These interpolating fields, being entire analytic functions of degree not greater than one and of type Λ, are also called quasicontinual fields. They may serve as an alternative for the existing approaches to field theories on lattices which emphasize momentum space or single sites pictures, and techniques. The quasicontinual approach takes full advantage of working with continuous functions in space–time. Functions of this sort form a quasicontinuum. This concept has several important applications already mentioned and promises to be useful in physics.

II. CONCEPT OF A QUASICONTINUUM

A. An interpolation problem

Let us start with the simplest example of a function of one variable $\Phi(x)$, $x \in R$.[1] Generalizations to higher dimensions will be obvious and corresponding final formulas will be given later.

We assume that the Fourier transform of $\Phi(x)$ has spectrum localized in the interval $[-\Lambda,\Lambda]$, $\Lambda = \pi/a$,

$$\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\Lambda}^{\Lambda} dp\, \tilde{\Phi}(p)\exp(ipx), \tag{1}$$

$$\tilde{\Phi}(p) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dx\, \Phi(x) \exp(-ipx). \qquad (2)$$

Expanding the function $\tilde{\Phi}(p)$ into the Fourier series and substituting into the first formula we get, after the integration over p,

$$\tilde{\Phi}(p) = \sum_{n=-\infty}^{\infty} C_n \exp(-inap), \quad p \in \mathfrak{A}, \qquad (3)$$

$$C_n = \frac{1}{2\Lambda} \int_{-\Lambda}^{\Lambda} dp\, \tilde{\Phi}(p) \exp(inap) = \frac{a}{\sqrt{2\pi}} \Phi(na), \qquad (4)$$

$$\Phi(x) = a \sum_{n=-\infty}^{\infty} \Phi(na) \delta_a(x - na), \qquad (5)$$

where the function $\delta_a(x)$ is given by the formula

$$\delta_a(x) = \frac{1}{2\pi} \int_{-\Lambda}^{\Lambda} dp \exp(ipx) = \frac{\sin(\Lambda x)}{\pi x}. \qquad (6)$$

Clearly, this function approaches the Dirac δ-function when $a \to 0$. Moreover, it shares most of the properties which we list here. The proofs are outlined in the Appendix

$$\delta_a(x) = \delta_a(-x) = \delta_a^*(x), \qquad (7a)$$

$$\delta_a(0) = a^{-1}, \qquad (7b)$$

$$\delta_a(na) = 0, \quad \text{for } n \neq 0, \qquad (7c)$$

$$\int_{-\infty}^{\infty} dx\, \delta_a(x) = 1, \qquad (7d)$$

$$\int_{-\infty}^{\infty} dx\, \delta_a(x - y) \Phi(x) = \Phi(y), \qquad (7e)$$

$$\int_{-\infty}^{\infty} dx\, \delta_a(x - ma) \delta_a(x - na) = \delta_{mn}, \qquad (7f)$$

$$a \sum_{n=-\infty}^{\infty} \delta_a(x - na) \delta_a(y - na) = \delta_a(x - y), \qquad (7g)$$

$$a \sum_{n=-\infty}^{\infty} \delta_a(x - na) = 1, \qquad (7h)$$

$$\lim_{a \to 0} \delta_a(x) = \delta(x). \qquad (7i)$$

Using property 7f of the δ_a-function, and formula (4), we get from formula (5) the equality

$$\int_{-\infty}^{\infty} dx\, \Phi(x) \delta_a(x - na) = \frac{\sqrt{2\pi}}{a} C_n = \Phi(na) \equiv \Phi_n. \qquad (8)$$

Therefore, if one introduces the equidistant lattice in R^1

$$x = na, \quad n \text{ integer}, \qquad (9)$$

and considers values of a function $\Phi(x)$ at lattice sites as given, one may recover it, or its Fourier transform, from the basic formulas

$$\Phi(x) = a \sum_{n=-\infty}^{\infty} \Phi_n \delta_a(x - na), \qquad (10)$$

$$\tilde{\Phi}(p) = \frac{a}{\sqrt{2\pi}} \sum_{n=-\infty}^{\infty} \Phi_n \exp(-inap). \qquad (11)$$

Conversely, when the functions $\Phi(x)$ or $\tilde{\Phi}(p)$ are known, we may find their lattice values as follows:

$$\Phi_n = \int_{-\infty}^{\infty} dx\, \Phi(x) \delta_a(x - na), \qquad (12)$$

$$\Phi_n = \frac{1}{\sqrt{2\pi}} \int_{-\Lambda}^{\Lambda} dp\, \tilde{\Phi}(p) \exp(inap). \qquad (13)$$

We have repeated some formulas here but we feel that it is worthwhile to collect the main expressions in a neat form as they constitute a backbone of what is called a quasicontinuum approach. The function $\Phi(x)$, being of the Fourier transform of a function with finite support, has special analytic properties which we shall discuss in the next section. Such functions compose the quasicontinuum which represents the discrete sets $\{\Phi(na), n \text{ integer}\}$. The function $\Phi(x)$ is also called the interpolating one for the set of its lattice values. The reason is that it agrees with *a priori* prescribed values $\Phi(na)$ at the lattice sites, when x approaches corresponding the site. This follows immediately from the properties (7b) and (7c) of the δ_a-function and formula (10), viz.,

$$\Phi(x)|_{x=na} = \Phi_n. \qquad (14)$$

For any two interpolating functions $\Phi_1(x)$, $\Phi_2(x)$ and their Fourier transforms $\tilde{\Phi}_1(p)$, $\tilde{\Phi}_2(p)$ we may write the Parseval relation, if they are square integrable functions,

$$\int_{-\infty}^{\infty} dx\, \Phi_1^*(x) \Phi_2(x) = \int_{-\Lambda}^{\Lambda} dp\, \tilde{\Phi}_1^*(p) \tilde{\Phi}_2(p) = a \sum_{n=-\infty}^{\infty} \Phi_{1_n}^* \Phi_{2n}. \qquad (15)$$

The last equality is a consequence of property 7f of the δ_a-function. Setting $\Phi_{1n} = 1$ and $\Phi_{2n} = \Phi_n$, we get, using formula (10) and property 7h of the δ_a-function, that the function $\Phi_1(x)$ is identically equal to unity. Hence the remarkable equality follows

$$\int_{-\infty}^{\infty} dx\, \Phi(x) = a \sum_{n=-\infty}^{\infty} \Phi_n. \qquad (16)$$

Formulas (15) and (16) show the perfect quality of interpolation with the function $\Phi(x)$ given by formula (10).

B. Uniqueness of interpolation and analyticity

In order to understand the somewhat miraculously unique correspondence between the set of lattice values $\{\Phi_n, n \in Z\}$ and interpolating functions $\Phi(x)$ one should realize that they may be analytically continued to entire functions of the variable $z = x + iy$

$$\Phi(z) = \frac{1}{\sqrt{2\pi}} \int_{-\Lambda}^{\Lambda} dp \exp(ipz) \tilde{\Phi}(p). \qquad (17)$$

Clearly, one may expand such a function into the Taylor series for any z. Moreover, due to the square integrability of $\tilde{\Phi}(p)$, one has the estimate

$$|\Phi(z)| \leqslant C \exp(\Lambda |y|). \qquad (18)$$

Therefore, it is the entire analytic function of degree not higher than one and of the type Λ. It is a theorem that the interpolation problem within the class of entire analytic function of degree not higher than one and of type Λ, and square integrable on a real axis, has a unique solution given by the formula

$$\Phi(z) = \sum_{n=-\infty}^{\infty} \Phi_n \frac{\sin \Lambda (z - n\pi/\Lambda)}{\Lambda (z - n\pi/\Lambda)}, \qquad (19)$$

and the series is uniformly convergent within every bounded region.[6] Clearly, for z real one recovers formula (10).

Having $\Phi(z)$ we also have at the same time all its derivatives at any point uniquely determined. The interpolating function $\Phi(z)$ representing the discrete set $\{\Phi_n; n\in Z\}$ of its lattice values, and having the above-mentioned analyticity properties in addition to square integrability, is an element of the quasicontinuum. The square integrability condition, although essential for the uniqueness of the interpolation problem, may be replaced by other conditions which will be discussed later. Concerning the functions $\Phi(x)$, we will also discuss the quasicontinual representations of discrete sets of their lattice values.

The functions $\Phi(x)$, $\tilde{\Phi}(p)$, and Φ_n may also be viewed as different representations (x,p, and n, respectively) of the single element of an abstract Hilbert space $\mathscr{H}$

$$\Phi(x) = \langle x|\Phi\rangle, \tag{20a}$$

$$\tilde{\Phi}(p) = \langle p|\Phi\rangle, \tag{20b}$$

$$\Phi_n = (1/\sqrt{a})\langle n|\Phi\rangle. \tag{20c}$$

Here $|x\rangle$, $|p\rangle$, and $|n\rangle$ are vectors of different orthogonal and complete bases in the space $\mathscr{H}$ (as a consequence of the Parseval relation)

$$\langle\Phi_1|\Phi_2\rangle = \int_{-\infty}^{\infty} dx\ \langle\Phi_1|x\rangle\ \langle x|\Phi_2\rangle \int_{-\Lambda}^{\Lambda} dp\ \langle\Phi_1|p\rangle\ \langle p|\Phi_2\rangle$$

$$= \sum_{n=-\infty}^{\infty} \langle\Phi_1|n\rangle\ \langle n|\Phi_2\rangle. \tag{21}$$

Assuming for the transition amplitudes between these bases the values

$$\langle x|p\rangle = \frac{\exp(ipx)}{\sqrt{2\pi}}, \tag{22a}$$

$$\langle n|x\rangle = \sqrt{a}\delta_a(x - na), \tag{22b}$$

$$\langle n|p\rangle = \left(\frac{a}{2\pi}\right)^{1/2}\exp(inap), \tag{22c}$$

we obtain the formulas (10)–(13) as unitary transformations from one basis to another.

C. Determination of derivatives at the lattice sites

The first derivative of the interpolating function may be readily calculated using formula A(6)

$$\Phi'_n = \frac{1}{\sqrt{2\pi}}\int_{-\Lambda}^{\Lambda} dp\ ip\tilde{\Phi}(p)\exp(inap) \tag{23a}$$

$$= a\sum_{m=-\infty}^{\infty} \Phi_n\delta'_a(ma - na) \tag{23b}$$

$$= \sum_{\substack{m=-\infty \\ m\neq n}}^{\infty} \frac{(-1)^{n-m}}{a(n-m)}\Phi_m. \tag{23c}$$

One immediately recognizes in it the celebrated SLAC derivative.[4] The highly nonlocal character of its dependence upon the field itself is evident. Every site but one contributes to it. One may calculate all other derivatives, in the same way, if needed.

D. Generalization to distributions

The whole construction may be generalized to the case when $\tilde{\Phi}(p)$ is a distribution of a compact support in $[-\Lambda,\Lambda]$. It is known that its Fourier transform $\Phi(x)$ is again an entire analytic function of degree not higher that one and of type Λ, and is polynomially bounded on a real axis.[11]

Let $N(\mathfrak{A})$ denote the space of test functions defined on the lattice sites $\{\varphi_n; n\in Z\}$ and which vanish, with $|n|$ going to infinity, faster than any inverse power of n, viz.

$$N(\mathfrak{A}) = \{\varphi_n; n^N\varphi_n \to 0 \text{ for all natural } N\}. \tag{24}$$

Let $P(\mathfrak{A})$ be the set of functions of the form

$$\tilde{\varphi}(p) = \frac{a}{\sqrt{2\pi}}\sum_{n=-\infty}^{\infty} \varphi_n\exp(-inap), \quad p\in\mathfrak{A}, \tag{25}$$

where $\varphi_n \in N(\mathfrak{A})$.

Further, let $X(\mathfrak{A})$ denote the Fourier transforms of elements from $P(\mathfrak{A})$ as given by the formula (1).

Let $P'(\mathfrak{A})$ be the set of distributions on the space $P(\mathfrak{A})$ defined by the formal series

$$\tilde{\Phi}(p) = \frac{a}{\sqrt{2\pi}}\sum_{n=-\infty}^{\infty} \Phi_n\exp(-inap), \quad p\in\mathfrak{A}, \tag{26}$$

where the coefficients $\Phi_n \in N'(\mathfrak{A})$ satisfy the polynomial bounds

$$|\Phi_n| \leqslant C|n|^N, \text{ for some natural number } N. \tag{27}$$

Finally, let $X'(\mathfrak{A})$ be the set of Fourier transforms of distributions from $P'(\mathfrak{A})$. For any $\varphi(x)\in X(\mathfrak{A})$ and $\Phi(x)\in X'(\mathfrak{A})$ we may write the equalities

$$(\Phi,\varphi) = \int_{-\infty}^{\infty} dx\ \Phi^*(x)\varphi(x) = \int_{-\Lambda}^{\Lambda} dp\ \tilde{\Phi}^*(p)\tilde{\varphi}(p)$$

$$= a\sum_{n=-\infty}^{\infty} \Phi_n^*\varphi_n. \tag{28}$$

The formulas (1), (2), and (10)–(13) are valid both for test functions and corresponding distributions, and establish the isomorphic mappings between the corresponding sets

$$N(\mathfrak{A}) \longleftrightarrow P(\mathfrak{A}) \longleftrightarrow X(\mathfrak{A}), \tag{29}$$

$$N'(\mathfrak{A}) \longleftrightarrow P'(\mathfrak{A}) \longleftrightarrow X'(\mathfrak{A}). \tag{30}$$

E. Uniqueness of the interpolation in the case of distributions

The question of uniqueness of the reconstruction of the distribution $\Phi(x)$ from Φ_n arises again since the square integrability property is now generally missing. The reconstruction will be unique if it yields zero distribution for the distribution $\Phi_{0n} \equiv 0$. Therefore, one first should examine whether the equations

$$\int_{\Lambda}^{\Lambda} dp\ \tilde{\Phi}_0(p)\exp(inap) = 0, \quad n\in Z, \tag{31}$$

admit some nonvanishing solutions for $\tilde{\Phi}_0(p)\in P'(\mathfrak{A})$. In fact, unfortunately, there exists a general solution of the form

$$\tilde{\Phi}_0(p) = \mathscr{P}\left(\frac{d}{dp}\right)[\delta(p-\Lambda) - \delta(p+\Lambda)], \tag{32}$$

where $\mathscr{P}(x)$ is a polynomial. This spoils the uniqueness of the interpolation procedure, since we have for $\Phi_0(x)$ the result

$$\Phi_0(x) = i\sqrt{\frac{2}{\pi}}\,\mathscr{P}(-ix)\sin(\Lambda x). \tag{33}$$

This function vanishes, however, at every lattice site. One sees that the uniqueness of interpolation holds when additional restrictions imposed on the function $\Phi(x)$ rule out the possibility of adding the funtion $\Phi_0(x)$ to $\Phi(x)$. This function vanishes, for instance, when $\Phi(x)$, and correspondingly $\Phi(na)$, is required to vanish at infinity. This is the case for the square integrable functions as considered in (IIB), and for the test functions belonging to $X(\mathfrak{A})$ in general. Any two interpolating distributions, corresponding to the same $\Phi(na)$, differ by a function of this form, and thus should be considered equivalent. Therefore, the uniqueness of the interpolation problem for the distributions, which also include functions as a special case, may be achieved by factorizing the space $X'(\mathfrak{A})$ over the linear subspace of functions of the form $\Phi_0(x)$. This can be effectively done by the identification of the end points of the set $\mathfrak{A}$. Indeed, one has in this case the equality

$$\delta(p-\Lambda) = \delta(p+\Lambda), \tag{34}$$

and the function $\tilde{\Phi}_0(p)$ vanishes identically. The set $\mathfrak{A}^*$, i.e., the set $\mathfrak{A}$ with identified end points, becomes equivalent to the circle of radius $r = \Lambda/\pi = a^{-1}$. It tends to the compactified line R^* when $a \to 0$, so it differs in topological properties from the usually considered momentum space R^1. Any momentum $p \in \mathfrak{A}^*$ may be viewed as a length of an arc of the circle $C(\Lambda/\pi)$ (see Fig. 1). The point $p = \Lambda + \delta$, $\delta > 0$, is equivalent to the point $p = -\Lambda + \delta$ if one is moving along the circle in the positive direction. Similarly, $p = -\Lambda - \delta$ is equivalent to the point $p = \Lambda - \delta$ when moving in the opposite direction. In this way any p may be represented on the circle $C(\Lambda/\pi)$. Clearly, the resulting momentum may be obtained from p by applying to it the operation mod 2Λ.

F. Operation of convolution

For any two distributions $\tilde{\Phi}_1(p)$, $\tilde{\Phi}_2(p)$ with supports in $\mathfrak{A}^*$ one may define their convolution $\tilde{\Phi}_1 * \tilde{\Phi}_2(p)$ with a support coinciding (this is essential) with the set $\mathfrak{A}^*$ again

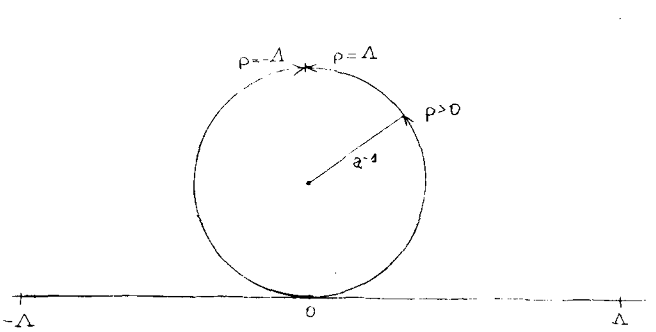

FIG. 1. Compactification of the interval $[-\Lambda, \Lambda]$ to the circle $C(\Lambda/\pi) = \mathfrak{A}$.

$$\tilde{\Phi}_1 * \tilde{\Phi}_2(p) = \int_{-\Lambda}^{\Lambda} dp'\,\tilde{\Phi}_1(p-p'|_{\mathrm{mod}\,2\Lambda})\tilde{\Phi}_2(p'). \tag{35}$$

This is not the case for the usual convolution operation, which doubles the support. Taking into account the equivalence of the points $\Lambda + \delta$ and $-\Lambda + \delta$ on the circle $C(\Lambda/\pi)$, one may derive the following useful formula for the convolution

$$\begin{aligned}\tilde{\Phi}_1 * \tilde{\Phi}_2(p) = \theta(p)\bigg[&\int_{-\Lambda}^{\Lambda-p} dp'\,\tilde{\Phi}_1(p+p')\tilde{\Phi}_2(-p')\\ &+ \int_{\Lambda-p}^{\Lambda} dp'\,\tilde{\Phi}_1(p+p'-2\Lambda)\tilde{\Phi}_2(-p')\bigg]\\ + \theta(-p)\bigg[&\int_{-\Lambda}^{-\Lambda-p} dp'\,\tilde{\Phi}_1(p+p'+2\Lambda)\tilde{\Phi}_2(-p')\\ &+ \int_{-\Lambda-p}^{\Lambda} dp'\,\tilde{\Phi}_1(p+p')\tilde{\Phi}_2(-p')\bigg].\end{aligned} \tag{36}$$

One infers from it the symmetry property

$$\tilde{\Phi}_1 * \tilde{\Phi}_2(p) = \tilde{\Phi}_2 * \tilde{\Phi}_2(p). \tag{37}$$

The convolution defined here coincides with the usual one when for at least one of the components $\tilde{\Phi}_1$ or $\tilde{\Phi}_2$ the following equality holds:

$$\tilde{\Phi}(p-p'|_{\mathrm{mod}\,2\Lambda}) = \tilde{\Phi}(p-p'), \text{ for all } p' \in \mathfrak{A}^*. \tag{38}$$

This is satisfied, clearly, in the following case:

(1) Momentum p is zero.

(2) $\tilde{\Phi}_1$ or $\tilde{\Phi}_2$ has support localized at $p' = 0$.

(3) $\tilde{\Phi}_1$ or $\tilde{\Phi}_2$ is a periodic function with the period 2Λ.

(4) $\tilde{\Phi}_1$ or $\tilde{\Phi}_2$ is a constant function, independent of p.

The convolution operation is a linear in every component, is symmetric, and has the property

$$(\tilde{\Phi}_1 * \tilde{\Phi}_2) * \tilde{\Phi}_3(p) = \tilde{\Phi}_1 * (\tilde{\Phi}_2 * \tilde{\Phi}_3)(p). \tag{39}$$

G. Multiplication of distributions

Let Φ_{1n}, Φ_{2n} be two distributions from $N'(\mathfrak{A}^*)$ and let $\Phi_1(x)$, $\Phi_2(x)$ be their interpolations belonging to $X'(\mathfrak{A}^*)$. Correspondingly, $\tilde{\Phi}_1(p)$, $\tilde{\Phi}_2(p)$ are their Fourier transforms, forming the set $P'(\mathfrak{A}^*)$. The product

$$\Phi_n = \Phi_{1n}\Phi_{2n} \tag{40}$$

does exist in $N'(\mathfrak{A}^*)$ since the polynomial bound is satisfied. Therefore, one may construct $\Phi(x)$ and $\tilde{\Phi}(p)$ for it. One easily finds, due to the periodicity property of exponential functions, the formula

$$\tilde{\Phi}_1 * \tilde{\Phi}_2(p) = a\sum_{n=-\infty}^{\infty} \Phi_{1n}\Phi_{2n}\exp(-inap). \tag{41}$$

Hence, according to (26), we have

$$\tilde{\Phi}(p) = (1/\sqrt{2\pi})\tilde{\Phi}_1 * \tilde{\Phi}_2(p) \tag{42}$$

and

$$\begin{aligned}\Phi(x) &= a\sum_{n=-\infty}^{\infty} \Phi_{1n}\Phi_{2n}\delta_a(x-na)\\ &= \frac{1}{\sqrt{2\pi}}\int_{-\Lambda}^{\Lambda} dp\,\exp(ipx)\tilde{\Phi}(p)\\ &= (1/2\pi)\int_{-\Lambda}^{\Lambda} dp\,\exp(ipx)\tilde{\Phi}_1 * \tilde{\Phi}_2(p).\end{aligned} \tag{43}$$

The distribution $\Phi(x)$ can be viewed as a kind of product of the distributions $\Phi_1(x)$, $\Phi_2(x)$ reconstructed from Φ_{1n} and Φ_{2n}, respectively. We shall denote this with a dot, while for the usual product the dot will be omitted

$$\Phi(x) = (\Phi_1 \cdot \Phi_2)(x) \in X'(\mathfrak{A}^*). \tag{44}$$

This is a commutative multiplication rule since the convolution of $\tilde{\Phi}_1$ and $\tilde{\Phi}_2$ is commutative. It differs, generally, from the usual product, since the convolution operation differs from the usual one, and it coincides with the usual product when the convolution does. According to the four cases considered in Sec. (II F), one can write the corresponding equalities

$$\begin{aligned}(1) \int_{-\infty}^{\infty} dx\, (\Phi_1^* \cdot \Phi_2)(x) &= \sqrt{2\pi}\,(\Phi_1^* \cdot \Phi_2)\tilde{\ }|_{(p=0)} \\ &= \tilde{\Phi}_1^*(-p) * \tilde{\Phi}_2(p)|_{p=0} \\ &= \int_{-\Lambda}^{\Lambda} dp\, \tilde{\Phi}_1^*(p)\tilde{\Phi}_2(p) \\ &= \int_{-\infty}^{\infty} dx\, \Phi_1^*(x)\Phi_2(x).\end{aligned} \tag{45}$$

$$(2)\ (\mathscr{P} \cdot \Phi)(x) = \mathscr{P}(x)\Phi(x) \text{ for any polynomial } \mathscr{P}. \tag{46}$$

$$(3)\ \delta_a(x-ma)\cdot\Phi(x) = \delta_a(x-ma)\Phi(x), \tag{47a}$$

$$\delta_a(x-ma)\cdot\delta_a(x-na) = a^{-1}\delta_{mn}\delta_a(x-ma). \tag{47b}$$

$$(4)\ (\delta_a \cdot \Phi)(x) = \delta_a(x)\Phi(x). \tag{48}$$

H. Violation of the Leibnitz rule

Let $\Phi(x)$ be the dot product of two distributions Φ_1 and Φ_2 defined according to (44). In order to calculate its derivative we apply the prescription (23) and the formula (42)

$$\Phi'(x) = (\Phi_1 \cdot \Phi_2)'(x) = \frac{1}{\sqrt{2\pi}} \int_{-\Lambda}^{\Lambda} dp\, ip\tilde{\Phi}(p)\exp(ipx) \tag{49}$$

$$\begin{aligned}&= \frac{i}{2\pi}\int_{-\Lambda}^{\Lambda} dp\, p\exp(ipx) \\ &\quad\times \int_{-\Lambda}^{\Lambda} dp'\, \tilde{\Phi}_1(p-p'|_{\text{mod}2\Lambda})\tilde{\Phi}_2(p').\end{aligned} \tag{50}$$

Using the identity

$$\begin{aligned}p &= p - p' + p' \\ &= p - p'|_{\text{mod}2\Lambda} + p' \\ &\quad + 2\Lambda\, [\theta(p-p'-\Lambda) - \theta(p'-p-\Lambda)],\end{aligned} \tag{51}$$

where θ is the usual step function, we may rewrite the last formula as follows

$$\begin{aligned}(\Phi_1\cdot\Phi_2)'(x) &= \frac{i}{2\pi}\int_{-\Lambda}^{\Lambda} dp\,\exp(ipx)\int_{-\Lambda}^{\Lambda} dp'\,(p-p'|_{\text{mod}2\Lambda})\tilde{\Phi}_1(p-p'|_{\text{mod}2\Lambda})\tilde{\Phi}_2(p') \\ &\quad+ \frac{i}{2\pi}\int_{-\Lambda}^{\Lambda} dp\,\exp(ipx)\int_{-\Lambda}^{\Lambda} dp'\tilde{\Phi}_1(p-p'|_{\text{mod}2\Lambda})p'\tilde{\Phi}_2(p') \\ &\quad+ \frac{i\Lambda}{\pi}\int_{-\Lambda}^{\Lambda} dp\,\exp(ipx)\int_{-\Lambda}^{\Lambda} dp'[\theta(p'-p-\Lambda)]\tilde{\Phi}_1(p-p'|_{\text{mod}2\Lambda})\tilde{\Phi}_2(p')\end{aligned} \tag{52}$$

$$= (\Phi_1'\cdot\Phi_2)(x) + (\Phi_1\cdot\Phi_2')(x) + \Delta_a(x,\Phi_1,\Phi_2). \tag{53}$$

Here the function $\Delta_a(x,\Phi_1,\Phi_2)$ measures the degree of violation of the Leibnitz rule. We shall call it the defect of the Leibnitz rule

$$\begin{aligned}\Delta_a(x,\Phi_1,\Phi_2) &= \frac{i\Lambda}{\pi}\int_{-\Lambda}^{\Lambda} dp\,\exp(ipx) \\ &\quad\times\int_{-\Lambda}^{\Lambda} dp'\,[\theta(p-p'-\Lambda)-\theta(p'-p-\Lambda)] \\ &\quad\tilde{\Phi}_1(p-p'|_{\text{mod}2\Lambda})\tilde{\Phi}_2(p').\end{aligned} \tag{54}$$

Clearly, the Leibnitz rule is satisfied in those cases when the dot product coincides with the usual one. In particular, according to the formula (46) of the previous section, we have for any polynomial $\mathscr{P}(x)$ and any distribution $\Phi(x) \in X'(\mathfrak{A}^*)$

$$(\mathscr{P}\cdot\Phi)'(x) = \mathscr{P}'(x)\Phi(x) + \mathscr{P}(x)\Phi'(x). \tag{55}$$

The function $\Delta_a(x,\Phi_1,\Phi_2)$ vanishes in the limit $a \to 0$, as one may easily see by applying the de l'Hospital's rule and using the equivalence of the end points in $\mathfrak{A}^*$

$$\begin{aligned}\lim_{a\to 0}\Delta_a(x,\Phi_1,\Phi_2) &= \lim_{a\to 0}\frac{i\pi}{a^2}\int_{-\infty}^{\infty} dp\,\exp(ipx) \\ &\quad\times\int_{-\infty}^{\infty} dp'\,[\delta(p'-p-\Lambda)-\delta(p'-p-\Lambda)]\tilde{\Phi}_1(p-p'|_{\text{mod}2\Lambda})\tilde{\Phi}_2(p') \equiv 0.\end{aligned} \tag{56}$$

Hence, the Leibnitz rule is restored in the continuum limit.

III. FORMFACTORS

The dot product of any two distributions may be equivalently written in the following way

$$(\Phi_1\cdot\Phi_2)(x) = (2\pi)^{-1}\int_{-\Lambda}^{\Lambda} dp' \int_{-\Lambda}^{\Lambda} dp'' \exp(ip'x)\tilde{\Phi}_1(p'-p''|_{\mathrm{mod}2\Lambda})\tilde{\Phi}_2(p'')$$

$$= \int_{-\infty}^{\infty} dx' \int_{-\infty}^{\infty} dx''\, M_a(x,x',x'')\Phi_1(x')\Phi_2(x''). \tag{57}$$

Here, the formfactor $M_a(x,x',x'')$ is given by its Fourier transform

$$M_a(x,x',x'') = (2\pi)^{-2}\int_{-\Lambda}^{\Lambda} dp' \int_{-\Lambda}^{\Lambda} dp'' \exp\{ip'x - i(p'-p''|_{\mathrm{mod}2\Lambda})x' - ip''x''\} \tag{58a}$$

$$= (2\pi)^{-2}\int_{-\Lambda}^{\Lambda} dp' \exp(ip'x)\exp(-ip'x') * \exp(-ip'x'') \tag{58b}$$

$$= (2\pi)^{-3/2}\int_{-\Lambda}^{\Lambda} dp \int_{-\Lambda}^{\Lambda} dp' \int_{-\Lambda}^{\Lambda} dp''\, \tilde{M}_a(p,p',p'')\exp(ipx + ip'x' + ip''x''), \tag{58c}$$

where

$$\tilde{M}_a(p,p',p'') = (2\pi)^{-1/2}\delta[p + (p'+p''|_{\mathrm{mod}2\Lambda})]. \tag{59}$$

The integral (58) can in fact be performed explicitly using the general formula (36) for a convolution and performing the integration over p'. After somewhat lengthy calculations one may arrive at the result

$$M_a(x,x',x'')$$
$$= \pi^{-2}\{[(x-x'')(x''-x')]^{-1}\sin(\Lambda x)\sin(\Lambda x') + [(x-x')(x-x'')]^{-1}\sin(\Lambda x')\sin(\Lambda x'') + [(x-x')(x''-x')]^{-1}\sin(\Lambda x)\sin(\Lambda x'')\}. \tag{60}$$

The following main properties of the formfactor can be readily seen from it or from the definition (58):

(1) $M_a(x,x',x'')$ is a completely symmetric function with respect to the permutation of its arguments.

(2) $M_a(x,x',x'')$ is a real function.

(3) $M_a(x,x',x'')$ is periodic under the simultaneous shift of all its variables by a lattice vector, viz.

$$M_a(x,x',x'') = M_a(x+na,x'+na,x''+na), \quad n\in Z. \tag{61}$$

(4) $$\int_{-\infty}^{\infty} dx\, M_a(x,x',x'') = \delta_a(x'-x''). \tag{62}$$

(5) $$\lim_{a\to 0} M_a(x,x',x'') = \delta(x-x')\delta(x'-x''). \tag{63}$$

The dot products of more than two fields lead to the formfactors of higher order. For instance, for the dot product of three fields we get, by applying the rule (57) twice

$$(\Phi_1\cdot\Phi_2\cdot\Phi_3)(x) = \int_{-\infty}^{\infty} dx'\, dx''\, dx'''\, M_a \times (x,x',x'',x''')\Phi_1(x')\Phi_2(x'')\Phi_3(x'''), \tag{64}$$

where the third order formfactor is

$$M_a(x,x',x'',x''')$$
$$= \int_{-\infty}^{\infty} dy\, M_a(x,x',y)M_a(y,x'',x''') \tag{65}$$
$$= (2\pi)^{-2}\int_{-\Lambda}^{\Lambda} dp\, dp'\, dp''\, dp'''\, \tilde{M}_a(p,p',p'',p''') \times\exp(ipx + ip'x' + ip''x'' + ip'''x'''), \tag{66}$$

where, furthermore,

$$\tilde{M}_a(p,p',p'',p''') = (2\pi)^{-1}\delta\{p + (p'+p''+p'''|_{\mathrm{mod}2\Lambda})\}. \tag{67}$$

Generally, for the dot product of n fields one gets

$$(\Phi_1\cdot\Phi_2\cdots\Phi_n)(x)$$
$$= \int_{-\infty}^{\infty} dx_1\cdots dx_n\, M_a(x,x_1,\ldots,X_n)\Phi_1(x_1)\cdots\Phi_n(x_n), \tag{68}$$

where the nth order formfactor is given by the formula

$$M_a(x,x_1,\ldots,x_n)$$
$$= \int_{-\infty}^{\infty} dy_1\cdots dy_{n-2}\, M_a(x,x_1,y_1)M_a \times(y_1,x_2,y_2)\cdots M_a(y_{n-2},x_{n-1},x_n) \tag{69}$$
$$= (2\pi)^{-n/2}\int_{-\Lambda}^{\Lambda} dp\, dp_1\cdots dp_n\, \tilde{M}_a(p,p_1,\ldots,p_n) \times\exp(ipx + ip_1x_1 + \cdots + ip_nx_n). \tag{70}$$

It is easily seen from this that it satisfies the recurrence relation

$$M_a(x,x_1,\ldots,x_n)$$
$$= \int_{-\infty}^{\infty} dy\, M_a(x,x_1,\ldots,x_{n-2},y)M_a(y,x_{n-1},x_n). \tag{71}$$

A similar formula holds for its Fourier transform

$$\tilde{M}_a(p,p_1,\ldots,p_n)$$
$$= (2\pi)^{-1/2}\int_{-\Lambda}^{\Lambda} dq\, \tilde{M}_a(p,p_1,\ldots,p_{n-2},-q) \times\delta[q + (p_{n-1}+p_n|_{\mathrm{mod}2\Lambda})]$$
$$= (2\pi)^{-(n-1)/2}\delta\left(p + \sum_{k=1}^{n}|_{\mathrm{mod}2\Lambda}p_k\right). \tag{72}$$

One can infer from this many properties of the formfactors, like their reality and full symmetry under the permutations of their arguments.

We have performed, actually, the integrations for the third order formfactor and we found, after some rather tedious calculations, the result

$$M_a(x,x',x'',x''')$$
$$= \pi^{-3}\{[(x-x')(x-x'')(x'''-x)]^{-1} \times\cos(\Lambda x)\sin(\Lambda x')\sin(\Lambda x'')\sin(\Lambda x''') + [(x-x')(x'-x'')(x'-x''')]^{-1}$$

$$\times\sin(\Lambda x)\cos(\Lambda x')\sin(\Lambda x'')\sin(\Lambda x''')$$
$$+\,[(x-x'')(x'-x'')(x'''-x'')]^{-1}$$
$$\times\sin(\Lambda x)\sin(\Lambda x')\cos(\Lambda x'')\sin(\Lambda x''')$$
$$+\,[(x-x''')(x'-x''')(x''-x''')]^{-1}$$
$$\times\sin(\Lambda x)\sin(\Lambda x')\sin(\Lambda x'')\cos(\Lambda x''')\}.$$

IV. EXPLICIT EXPRESSION FOR THE DEFECT OF THE LEIBNITZ RULE

Let us go back now to the formula (54) for the defect of the Leibnitz rule and write it in a slightly different form. Namely, upon performing the inverse Fourier transform on fields we get

$$\Delta_a(x,\Phi_1,\Phi_2)=\int_{-\infty}^{\infty}dx'\,dx''\,\Delta_a(x,x',x'')\Phi_1(x')\Phi_2(x''), \quad (73)$$

where the kernel function is

$$\Delta_a(x,x',x'')$$
$$=\frac{i\Lambda}{2\pi^2}\int_{-\Lambda}^{\Lambda}dp\,dp'\,[\theta(p+p'-\Lambda)-\theta(-p-p'-\Lambda)]$$
$$\times\exp\{ipx-i(p+p'|_{\mathrm{mod}2\Lambda})x'+ip'x''\}. \quad (74)$$

This function, and thus the whole defect $\Delta_a(x,\Phi_1,\Phi_2)$, may be expressed through the formfactor $M_a(x,x',x'')$. Indeed, the formula (53) for differentiation of product of two fields may be written as follows

$$\int_{-\infty}^{\infty}dx'\,dx''\,\frac{\partial}{\partial x}M_a(x,x',x'')\Phi_1(x')\Phi_2(x'')$$
$$=\int_{-\infty}^{\infty}dx'\,dx''\,M_a(x,x',x'')$$
$$\times[\Phi_1'(x')\Phi_2(x'')+\Phi_1(x')\Phi_2'(x'')]$$
$$+\int_{-\infty}^{\infty}dx'\,dx''\,\Delta_a(x,x',x'')\Phi_1(x')\Phi_2(x''). \quad (75)$$

Taking into account that $\Phi_k(x)$ are distributions and are of arbitrary form, we obtain from it the expression

$$\Delta_a(x,x',x'')=\left(\frac{\partial}{\partial x}+\frac{\partial}{\partial x'}+\frac{\partial}{\partial x''}\right)M_a(x,x',x''). \quad (76)$$

Using the explicit formula (60) for the formfactor, one gets the explicit formula for the kernel of the defect of the Leibnitz rule

$$\Delta_a(x,x',x'')=-(\Lambda/\pi^2)[(x-x')(x'-x'')(x''-x)]^{-1}$$
$$\times[(x-x')\sin(x+x')+(x'-x'')$$
$$\times\sin\Lambda(x'+x'')+(x''-x)\sin(x''+x)]. \quad (77)$$

One sees that it is a real and fully symmetric function.

V. GENERALIZATIONS TO HIGHER DIMENSIONS

The whole scheme presented so far permits obvious generalizations to higher—let us say D—dimensions. We shall list here only the main formulas, for the sake of completeness of the paper. In order to minimize necessary changes in the previous formulas we shall use the following compact notations:

$$x=(x^1,\dots,x^D)\in R^D. \quad (78)$$

$$n=(n^1,\dots,n^D),\quad n^\mu\in Z. \quad (79)$$

$$xp=x^\mu p_\mu\quad \mu=1,\dots,D. \quad (80)$$

$$\mathfrak{A}=\left\{p;\,-\Lambda\leqslant p_\mu\leqslant\Lambda,\quad \mu=1,\dots,D,\quad \Lambda=\frac{\pi}{a}\right\}. \quad (81)$$

$$\delta_a(x)=\prod_{\mu=1}^{D}\delta_a(x^\mu). \quad (82)$$

The Fourier transform of a distribution $\Phi(x)\in X'(\mathfrak{A})$ is defined naturally

$$\tilde\Phi(p)=(2\pi)^{-D/2}\int d^Dx\,\Phi(x)\exp(-ipx), \quad (83)$$

$$\Phi(x)=(2\pi)^{-D/2}\int_{\mathfrak{A}}d^Dp\,\tilde\Phi(p)\exp(ipx). \quad (84)$$

A distribution $\Phi(x)$ is called the interpolation of a set of lattice values $\{\Phi_n,\,n\in Z_D\}$ if the following formulas hold:

$$\Phi(x)=a^D\sum_n\Phi_n\delta_a(x-an), \quad (85)$$

$$\tilde\Phi(p)=(a^2/2\pi)^{D/2}\sum_n\Phi_n\exp(-ianp),\quad p\in\mathfrak{A} \quad (86)$$

$$\Phi_n=(2\pi)^{-D/2}\int_{\mathfrak{A}}d^Dp\,\tilde\Phi(p)\exp(ianp), \quad (87)$$

$$\Phi_n=\int d^Dx\,\delta_a(x-an)\Phi(x). \quad (88)$$

Uniqueness of the interpolation is achieved by the identification of endpoints of the D-dimensional cube $\mathfrak{A}$, yielding the set $\mathfrak{A}^*$.

The convolution operation is defined as

$$\tilde\Phi_1*\tilde\Phi_2(p)=\int_{\mathfrak{A}^*}d^Dp\,\tilde\Phi_1(p-p'|_{\mathrm{mod}2\Lambda})\tilde\Phi_2(p'), \quad (89)$$

where for brevity we put

$$p-p'|_{\mathrm{mod}2\Lambda}=\{p_\mu-p'_\mu|_{\mathrm{mod}2\Lambda},\quad \mu=1,\dots,D\}. \quad (90)$$

The product of two distributions

$$\Phi_n=\Phi_{1n}\Phi_{2n} \quad (91)$$

generates, through (84) and (85), the distribution

$$\Phi(x)=a^D\sum_n\Phi_{1n}\Phi_{2n}\delta_a(x-an) \quad (92)$$
$$=(2\pi)^{-D}\int_{\mathfrak{A}^*}d^Dp\,\exp(ipx)\tilde\Phi_1*\tilde\Phi_2(p)\equiv(\Phi_1\cdot\Phi_2)(x) \quad (93)$$

$$=\int d^Dx'\int d^Dx''\,M_a(x,x',x'')\Phi_1(x')\Phi_2(x''), \quad (94)$$

where the formfactor is simply the product of the one-dimensional formfactors

$$M_a(x,x',x'')=\prod_{\mu=1}^{D}M_a(x^\mu,x'^\mu,x''^\mu). \quad (95)$$

For the differentiation rule of the product we get the rule

$$\partial_\mu(\Phi_1\cdot\Phi_2)(x)=(\partial_\mu\Phi_1\cdot\Phi_2)(x)$$
$$+(\Phi_1\cdot\partial_\mu\Phi_2)(x)+\Delta_{a\mu}(x,\Phi_1,\Phi_2), \quad (96)$$

where the defect of the Leibnitz rule is

$$\Delta_{a\mu}(x,\Phi_1,\Phi_2)$$
$$= \frac{i\Lambda}{\pi(2\pi)^{D-1}}\int_{\mathfrak{N}^*} d^Dp\,\exp(ipx)$$
$$\times\int_{\mathfrak{N}^*} dp'\,[\theta(p_\mu - p'_\mu - \Lambda) - \theta(p'_\mu - p_\mu - \Lambda)]$$
$$\times\tilde{\Phi}_1(p - p'|_{\mathrm{mod}2\Lambda})\tilde{\Phi}_2(p')$$
$$= \int d^Dx' \int d^Dx''\,\Delta_{a\mu}(x,x',x'')\Phi_1(x')\Phi_2(x''), \tag{97}$$

where the kernel is given by the formulas

$$\Delta_{a\mu}(x,x',x'')$$
$$= \frac{i\Lambda}{\pi(2\pi)^{2D-1}}\int_{\mathfrak{N}^*} d^Dp\,\exp(ipx)\int_{\mathfrak{N}^*} d^Dp'\,[\theta(p_\mu - p'_\mu - \Lambda) \tag{98a}$$
$$- \theta(p'_\mu - p_\mu - \Lambda)]\exp(-i(p - p'|_{\mathrm{mod}2\Lambda})x' - ip'x'')$$
$$= \left(\frac{\partial}{\partial x^\mu} + \frac{\partial}{\partial x'^\mu} + \frac{\partial}{\partial x''^\mu}\right)M_a(x,x',x'') \tag{98b}$$
$$= M_a(x,x',x'')[\Delta_a(x_\mu,x'_\mu,x''_\mu)]/M_a(x^\mu,x'^\mu,x''^\mu). \tag{98c}$$

VI. CONCLUDING REMARKS

The next problem, after developing the above formalism, is mainly applications to a field theory on a lattice. One may think of a lattice introduced in all the space–time variables or only in the spatial ones. Both may be treated in the same way. In subsequent publications we shall present corresponding calculations. We shall remark here only that a field theory written in terms of the quasicontinual field is a nonlocal one. The relevant formfactors were studied in the Sec. III.

The theory presented is, of course, quite universal and may be applied to any set of discrete quantities, like spins at lattice sites, etc. It permits the equivalent, quasicontinual, representation of this set in the position space, which might be useful.

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APPENDIX: PROOFS OF THE PROPERTIES (7a)–(7l) OF THE δ_a-FUNCTION

The property (7a) is evident from the formula (6). The same is true for the properties (7c), (7d), and (7i). The property (7b) follows from l'Hospital's rule

$$\delta_a(0) = \lim_{x\to 0}[\sin(\Lambda x)/\pi x] = \Lambda/\pi = a^{-1}. \tag{A1}$$

The property (7e) may be verified by substituting $\varphi_1(x) = \delta_a(x-y)$ and $\varphi_2(x) = \varphi(x)$ into the Parseval relation A(15). Indeed, we have in this case

$$\tilde{\varphi}_1(p) = \frac{\exp(-ipy)}{\sqrt{2\pi}}, \quad \tilde{\varphi}_2(p) = \tilde{\varphi}(p), \tag{A2}$$

and the Parseval relation reads

$$\int_{-\infty}^{\infty} dx\,\delta_a(x-y)\varphi(x) = \frac{1}{\sqrt{2\pi}}\int_{-\Lambda}^{\Lambda} dp\,\tilde{\varphi}(p)\exp(ipy)$$
$$= \varphi(y). \tag{A3}$$

The property (7f) follows from (7e), together with the properties (7b) and (7c), because the function $\delta_a(x)$ is a permissible one as the Fourier transform of a function of compact support.

The property (7g) is a consequence of the well-known summation formula[10]

$$\sum_{n=-\infty}^{\infty}\exp(inap) = \frac{2\pi}{a}\sum_{n=-\infty}^{\infty}\delta\left(p - \frac{2\pi}{a}n\right). \tag{A4}$$

The property (7h) follows from (7g) upon the integration over x. Thus all the listed properties of the δ_a-function are verified.

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The n-bubble diagram contribution to g-2

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We obtain an exact integrated expression for the contribution of the mass-independent n-bubble diagram to the leptonic g-2. Furthermore, we find an interesting pattern of zeroes among the coefficients of the zeta functions which occur in the result. This pattern also occurs when we generalize to integrals of the same type as the one occurring in the n-bubble diagram. We explain this pattern in a theorem which we rigorously prove.

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I. INTRODUCTION

In spite of the steady increase in the number and accuracy of the experimental tests, quantum electrodynamics (QED) continues to meet each new challenge successfully.[1] In recent years, much interest has focused on studying the asymptotic behavior in N of the Nth order perturbation expansion.[2] Not only does the number of diagrams[3] contributing grow rapidly with N, but there are single diagrams which contribute factorial growth to amplitudes. In particular, Lautrup[4] has shown that the n-bubble diagram contributes, in a gauge-invariant way, to the anomalous magnetic moment of the electron $a_n = (g-2)/2$ like $n!$ and, as a result, these contributions are not Borel-summable.

In spite of its tremendous successes, there are still questions that remain unanswered in QED. As far back as the Twelfth Solvay Congress in 1960, R.P. Feynman issued a call for further intuition and insight into the calculations in QED and new approaches to old problems.[5] The question of whether or not there is a completely finite theory[6] will not be addressed here. Other questions are these.

(1) Can one determine the sign or estimate the magnitude of an amplitude without a complete calculation?

(2) Can one understand the tremendous cancellations that typically occur in adding the contributions from different gauge-invariant classes of graphs, as well as within the expression for a single class?

(3) Is there perhaps a better, mathematically more efficient way of expressing the amplitudes?

Here we report on a modest contribution towards addressing these very difficult questions. We obtain an exact integrated expression for the contribution of the mass-independent n-bubble diagram to the leptonic g-2.[7]

The motivation for studying this diagram, is that the anomaly a_n, in this case, can be done exactly to all orders and that the questions (1) and (2) above can be partly answered. We find that the coefficients of some of the zeta functions in the result become zero if n is sufficiently large. We will study these zeroes in detail and explain why they arise. a_n is given by a multiple sum over binomial coefficients and Stirling numbers of the first kind, and it is the identification of a_n in terms of these Stirling numbers which makes the problem tractable. To our knowledge, this is the first time an exact treatment in Nth order perturbation theory has been done.

This report is organized as follows: In Sec. II, we give the exact integrated form of a_n. The details leading to this are given in appendices A, B, and C. Using the algebraic program REDUCE,[8] a_n is then calculated explicitly up to $n = 13$, that is 13 bubbles.

Section III is devoted to two simple examples, both having all the properties of a_n. In these examples the pattern of vanishing $\zeta(l)$ coefficients will become clear.

Finally in Sec. IV we generalize to integrals of the type occurring in a_n. First we prove the pattern of zeroes among the $\zeta(l)$ terms for a_n, and then the proof is generalized to other integrals.

II. EXPRESSIONS FOR $\bar{Z}(n,l)$ AND $R(n)$

The contribution of Fig. 1 to g-2 is given by[4]

$$a_n = \frac{1}{3^n}\int_0^1 dx(1-x)\,[f(x)]^n, \tag{1}$$

with

$$f(x) = -\frac{5}{3} - \frac{4}{x} + \frac{4}{x^2} + \left(1 - \frac{6}{x^2} + \frac{4}{x^3}\right)\log(1-x). \tag{2}$$

Since $f(x) \to 0$ for $x \to 0$, a_n is finite. After binomial expansion of $[f(x)]^n$ and using Eq. (C6) (see Appendix C), a_n becomes

$$\left(\frac{1}{3}\right)^n \sum \binom{n}{i}\left(-\frac{5}{3}\right)^i \binom{i}{i_1}\left(\frac{12}{5}\right)^{i_1}\binom{i_1}{i_2}(-1)^{i_2} \times \binom{n-i}{i_3}(-6)^{i_3}\binom{i_3}{i_4}\left(-\frac{2}{3}\right)^{i_4} \times \{I_\epsilon(n-i, m-1) - I_\epsilon(n-i, m-2)\}, \tag{3}$$

with $m \equiv i_1 + i_2 + 2i_3 + i_4$ and the limits on the sum are given by $0 \leqslant i_2 \leqslant i_1 \leqslant i \leqslant n$ and $0 \leqslant i_4 \leqslant i_3 \leqslant n - i$. The integral $I_\epsilon(n,m)$ is defined in the limit $\epsilon \to 0$:

$$I_\epsilon(n,m) \equiv \int_\epsilon^1 \frac{\log^n(1-x)}{x^{m+1}}\,dx, \quad n, m = 0,1,2,\cdots. \tag{4}$$

$I_\epsilon(n,m)$ is a sum of a divergent part $D_\epsilon(n,m)$, a finite term $Z(n,m)$ consisting of Riemann zeta functions with rational coefficients and a finite rational term $R(n,m)$.

$$I_\epsilon(n,m) = D_\epsilon(n,m) + Z(n,m) + R(n,m). \tag{5}$$

The easiest way to obtain D_ϵ is to expand [see Eq. (A3)]

$$\log^n(1-x) = (-1)^n n! \sum_{k=n}^{\infty} \frac{1}{k!}\left[{n \atop k}\right] x^k, \tag{6}$$

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where we define $\left[{n \atop m}\right] \equiv |S_m^{(n)}|$; $S_m^{(n)}$ being the Stirling numbers of the first kind.[9] The numbers $\left[{n \atop m}\right]$ are nonnegative integers which obey the recursion relation

$$\begin{bmatrix} n \\ m+1 \end{bmatrix} = \begin{bmatrix} n-1 \\ m \end{bmatrix} + m \begin{bmatrix} n \\ m \end{bmatrix}, \tag{7}$$

with $\left[{n \atop m}\right] = 0$ if $m < n$ and $\left[{n \atop n}\right] = 1$. Using Eqs. (4), (5), and (6), or equivalently, Eq. (A7), we find

$$D_\epsilon(n, m) = (-1)^n n! \left\{ \frac{1}{m!} \begin{bmatrix} n \\ m \end{bmatrix} (-\log \epsilon) + \sum_{k=1}^{n-m} \frac{1}{k(m-k)!} \begin{bmatrix} n \\ m-k \end{bmatrix} \frac{1}{\epsilon^k} \right\}. \tag{8}$$

To find the Z and R part, we have for $n \geqslant 1$, $m = 0$ [see Eqs. (A8) and (A9)]

$$I_\epsilon(n,0) = \int_0^1 dx \frac{\log^n(1-x)}{x} = (-1)^n n! \zeta(n+1),$$

with

$$\zeta(n) \equiv \sum_{k=1}^{\infty} \frac{1}{k^n}, \tag{9}$$

or $Z(n,0) = (-1)^n n! \zeta(n+1)$ and $R(n,0) = 0$. If $n,m \geqslant 1$, we find, after a partial integration on x^{-m-1} [see Eq. (A12)],

$$I_\epsilon(n, m) = (-1)^n \frac{n!}{m} \sum_{k=n}^{m-1} \frac{1}{k!} \begin{bmatrix} n \\ k \end{bmatrix} \frac{1}{\epsilon^{m-k}} + (-1)^n \frac{n!}{m m!} \begin{bmatrix} n \\ m \end{bmatrix} + (-1)^n \frac{n!}{m} \zeta(n) - \frac{n}{m} \sum_{i_1=1}^{m-1} I_\epsilon(n-1, i_1). \tag{10}$$

Equations (5) and (10) give the two recursion-relations

$$Z(n,m) = (-1)^n \frac{n!}{m} \zeta(n) - \frac{n}{m} \sum_{i_1=1}^{m-1} Z(n-1, i_1), \tag{11}$$

and

$$R(n, m) = (-1)^n \frac{n!}{m m!} \begin{bmatrix} n \\ m \end{bmatrix} - \frac{n}{m} \sum_{i_1=1}^{m-1} R(n-1, i_1), \tag{12}$$

with

$$R(1,m) = -\frac{1}{m^2} + \frac{1}{m!} \begin{bmatrix} 2 \\ m \end{bmatrix}.$$

Using Eq. (11) recursively $n-2$ times, one obtains [for details see Eqs. (A14)–(A18)]

$$Z(n, m) = (-1)^n \frac{n!}{m!} \sum_{k=0}^{n-1} \zeta(n+1-k) \begin{bmatrix} k \\ m \end{bmatrix}, \quad m \geqslant 0. \tag{13}$$

Similarly, using Eq. (12) recursively, $n-2$ times, one finds [for details see Eqs. (A19)–(A23)]

$$R(n,m) = (-1)^{n+1} \frac{n!}{m!} \begin{bmatrix} n+1 \\ m \end{bmatrix} + (-1)^n \frac{n!}{(m!)^2} \left[\!\!\begin{bmatrix} n \\ m \end{bmatrix}\!\!\right], \quad \text{if } m \geqslant 0. \tag{14a}$$

If $m < 0$, one finds easily from Eq. (4)

$$R(n,m) = (-1)^n n! \sum_{i=0}^{-1-m} (-1)^i \binom{-l-m}{i} \frac{1}{(1+i)^{n+1}}. \tag{14b}$$

The numbers $\left[\!\left[{n \atop m}\right]\!\right]$ which show some similarities to $\left[{n \atop m}\right]$ are also nonnegative integers and satisfy the recursion relation

$$\left[\!\!\begin{bmatrix} n \\ m+1 \end{bmatrix}\!\!\right] = (m+1) \left[\!\!\begin{bmatrix} n-1 \\ m \end{bmatrix}\!\!\right] + m(m+1) \left[\!\!\begin{bmatrix} n \\ m \end{bmatrix}\!\!\right] + m \begin{bmatrix} 1 \\ m \end{bmatrix} \left\{ \begin{bmatrix} n-1 \\ m \end{bmatrix} - \begin{bmatrix} n \\ m \end{bmatrix} \right\}, \tag{15}$$

with

$$\left[\!\!\begin{bmatrix} n \\ m \end{bmatrix}\!\!\right] = 0 \quad \text{if } m < n,$$

$$\left[\!\!\begin{bmatrix} n \\ n \end{bmatrix}\!\!\right] = \begin{bmatrix} 2 \\ n+1 \end{bmatrix},$$

and

$$\left[\!\!\begin{bmatrix} 1 \\ m \end{bmatrix}\!\!\right] = \begin{bmatrix} 1 \\ m \end{bmatrix}^2.$$

TABLE I. $\tilde{Z}(n,l)$, the coefficient of $\zeta(l)$ in a_n. Note that for $l > n+1$, $\tilde{Z}(n,l)$ vanishes trivially [See Eqs. (7) and (11)].

$n \backslash l$	2	3	4	5	6	7	8	9
1	-2							
2	$-\frac{8}{45}$	$\frac{8}{3}$						
3	0	$\frac{32}{63}$	-4					
4	0	$-\frac{128}{675}$	$-\frac{43856}{31185}$	$\frac{64}{9}$				
5	0	0	$\frac{39344}{35721}$	$\frac{83360}{22113}$	$-\frac{400}{27}$			
6	0	0	$-\frac{512}{14175}$	$\frac{1119488}{280665}$	$-\frac{15136640}{1378377}$	$\frac{320}{9}$		
7	0	0	$-\frac{896}{91125}$	$-\frac{130048}{382725}$	$\frac{66764848}{4691115}$	$\frac{68084800}{1980693}$	$-\frac{7840}{81}$	
8	0	0	0	$\frac{16384}{54675}$	$\frac{3625958144}{940355325}$	$-\frac{949387578112}{18422008605}$	$-\frac{273363470080}{2323352889}$	$\frac{71680}{243}$

In principle, we can forget about the D_ϵ term, since a_n is finite and these terms therefore have to cancel in the final sum. However, the divergent parts play a crucial role in our proof of the pattern of zeroes of the $\zeta(l)$ coefficients. We will return to these D_ϵ in Sec. IV. From Eqs. (3), (4), (5), (13), and (14) we obtain

$$a_n = \sum_{l=2}^{n+1} \widetilde{Z}(n,l)\zeta(l) + R(n). \qquad (16)$$

The coefficient of $\zeta(l)$ is

$$\widetilde{Z}(n,l) = (-1/3)^n n! \sum \frac{1}{i!}\left(\frac{5}{3}\right)^i \binom{i}{i_1}\left(\frac{12}{5}\right)^{i_1}\binom{i_1}{i_2}(-1)^{i_2} \times \binom{n-i}{i_3}(-6)^{i_3}\binom{i_3}{i_4}\left(-\frac{2}{3}\right)^{i_4} \times \left\{\frac{1}{(m-1)!}\begin{bmatrix} n+1-l-i \\ m-1 \end{bmatrix} - \frac{1}{(m-2)!}\begin{bmatrix} n+1-l-i \\ m-2 \end{bmatrix}\right\}, \qquad (17)$$

with m defined as in Eq. (3) and the limits on the sum given by $0 \leqslant i_2 \leqslant i_1 \leqslant i \leqslant n+1-l$ and $0 \leqslant i_4 \leqslant i_3 \leqslant n-i$. Although this formula looks complicated, for $l = n+1$ it simplifies to

$$\widetilde{Z}(n,n+1) = (-1)^n (n!/3^n)(6n). \qquad (18)$$

Notice, this increases much faster with n than does a_n,[4]

$$a_n \sim e^{-10/3} n!/(2 \times 6^n) \qquad (19)$$

To arrive at Eq. (17), it has been convenient to change the double sum [see Eq. (C8)],

$$\sum_{i=0}^{n-1} \sum_{k=0}^{n-1-i} \zeta(n+1-i-n) \begin{bmatrix} k \\ m \end{bmatrix},$$

into the double sum

$$\sum_{l=2}^{n+1} \zeta(l) \sum_{i=0}^{n+1-l} \begin{bmatrix} n+1-l-i \\ m \end{bmatrix}.$$

In this way we can pick out a specific $\zeta(l)$ term. For the rationals $R(n)$ we obtain

$$R(n) = \frac{1}{3^n} \sum \binom{n}{i}\left(-\frac{5}{3}\right)^i \binom{i}{i_1}\left(\frac{12}{5}\right)^{i_1}\binom{i_1}{i_2}(-1)^{i_2} \times \binom{n-i}{i_3}(-6)^{i_3}\binom{i_3}{i_4}\left(-\frac{2}{3}\right)^{i_4} \times \{R(n-i, m-1) - R(n-i, m-2)\}, \qquad (20)$$

with the limits on the sum given by $0 \leqslant i_2 \leqslant i_1 \leqslant i \leqslant n$ and $0 \leqslant i_4 \leqslant i_3 \leqslant n-i$ [m as in Eq. (3)]. The problem of calculating a_n has now been reduced to evaluating the summations in Eqs. (17) and (20). To do this we have used the algebraic program REDUCE.[8] In Table I we give $\widetilde{z}(n,l)$ for $n \leqslant 8$. In Table II we continue $\widetilde{Z}(n,l)$ for $9 \leqslant n \leqslant 13$, $5 \leqslant l \leqslant 10$. Finally, Table III continues $\widetilde{z}(n,l)$ for $9 \leqslant n \leqslant 13$, $11 \leqslant l \leqslant 14$.

Table IV contains $R(n)$ for $n \leqslant 13$. The results agree with Samuel, Caffo *et al.*,[10] and Lautrup,[4] wherever comparison is possible. In principle we can go on with higher n, but the amount of computer time needed increases rapidly ($\sim n^5$). For example, calculating $\widetilde{Z}(13,l)$ for $l = 2, 14$ took about 5 hours c.p.u. time on an IBM 360/158. From Tables I, II, and III, one notices that

TABLE II. $\widetilde{Z}(n,l)$, the coefficient of $\zeta(l)$ in a_n continuation. The entries for $l = 2,3,4$ are zero and have been omitted to save space.

$n \backslash l$	5	6	7	8	9	10
9	$-\frac{57344}{2278125}$	$-\frac{439536128}{147349125}$	$\frac{17070662656}{689593905}$	$\frac{19972941378688}{101116358343}$	$\frac{24440824832}{56119635}$	$-\frac{8960}{9}$
10	0	$\frac{5761024}{1722625}$	$\frac{249123798016}{14481472005}$	$\frac{1934791448782592}{13230686580111}$	$-\frac{1291228747857920}{1610083552077}$	$-\frac{353266892815360}{202131701343}$
11	0	$\frac{90112}{6834375}$	$\frac{815276032}{1808375625}$	$-\frac{9364674206471296}{99704934754425}$	$-\frac{17449844608302592}{21322180852245}$	$\frac{37074849201664}{10678036005}$
12	0	$-\frac{720896}{307546875}$	$-\frac{1657339904}{1291696875}$	$-\frac{16278130970624}{691161163875}$	$\frac{903633874895839232}{1894393760334075}$	$\frac{4617319876279752826 88}{98899382186329725}$
13	0	0	$\frac{37486592}{184528125}$	$\frac{33447130062848}{1708914965625}$	$\frac{1485098236830023 68}{575220777429375}$	$-\frac{612343786554451779328}{2537373289576 87575}$

TABLE III. $\widetilde{Z}(n,l)$, the coefficient of $\zeta(l)$ in a_n continuation.

$n \backslash l$	11	12	13	14
9				
10	$\frac{896000}{243}$			
11	$\frac{444304627283968}{58928677821}$	$-\frac{10841600}{729}$		
12	$-\frac{2250198084493426 81088}{14071398388992945}$	$-\frac{19901585596856320}{569643885603}$	$\frac{15769600}{243}$	
13	$-\frac{370035019211740346368}{13693760610414885}$	$\frac{345633587031276698 74688}{441375638225157405}$	$\frac{2521170633435271168}{14591647223523}$	$-\frac{666265600}{2187}$

$$\widetilde{Z}(n,2) = 0 \quad \text{for } n \geqslant 3,$$
$$\widetilde{Z}(n,3) = 0 \quad \text{for } n \geqslant 5,$$
$$\widetilde{Z}(n,4) = 0 \quad \text{for } n \geqslant 8, \tag{21}$$
$$\widetilde{Z}(n,5) = 0 \quad \text{for } n \geqslant 10,$$
$$\widetilde{Z}(n,6) = 0 \quad \text{for } n \geqslant 13.$$

One, therefore, suspects that there is a general rule for the pattern of zeroes for $\widetilde{Z}(n,l)$. Here we state the general rule as follows (the proof of this will be given in Sec. IV). Let

$$f(x) = P(x) + Q(x)\log(1-x),$$

where

$$P(x) = \sum_{i=0}^{s-1} \frac{p_i}{x^i} \tag{22}$$

and

TABLE IV. R(n), the rational term in a_n.

n	$R(n)$
1	$\frac{119}{36}$
2	$-\frac{943}{324}$
3	$\frac{151849}{40824}$
4	$-\frac{3689383}{656100}$
5	$\frac{428632663}{42987672}$
6	$-\frac{23973913987}{1169170200}$
7	$\frac{8807062662626447}{181934574822000}$
8	$-\frac{3657842896431364117}{28202252973394500}$
9	$\frac{299105349780987278087089}{767229472935300375000}$
10	$-\frac{508941309402135235540 0597}{39132385821170408566 80}$
11	$\frac{19984867920592543211435106797}{41892905364045180599 70000}$
12	$-\frac{346169238107153153686623992774 6623}{181381752847842616329234975000}$
13	$\frac{154163936497731065583646798434060 20749}{186393141910688439927906055350000}$

$$Q(z) = \sum_{i=0}^{s} \frac{q_i}{x^i}, \quad s = 1,2,\ldots;$$

p_i, q_i are rational numbers. Furthermore, let $f(x) \to x^r$ as $x \to 0, r = 0,1,2\cdots$. Then the $\xi(1)$ coefficient in the integral

$$\int_0^1 dx\, x^t [f(x)]^n, \quad t = 0,1,2,\cdots$$

vanishes whenever

$$rn \geqslant (r+s)(l-1) - t. \tag{23}$$

For the n-bubble diagram we have $r = 2$, $s = 3$, and $t = 0$ and 1 [see Eq. (1)]. Equation (23), in this case, yields

$$2n \geqslant 5l - 5 \quad \text{for } t = 0$$

and (24)

$$2n \geqslant 5l - 6 \quad \text{for } t = 1.$$

For instance, $l = 2$, $t = 0$ implies $n \geqslant 2.5$ or, since n is an integer $n \geqslant 3$, $t = 1$ gives $n \geqslant 2$. Now, since both conditions must be satisfied, $n \geqslant 3$. By inspection, we find from Eq. (24) that the rest of Eq. (21) is satisfied. The rule mentioned in Eq. (23) now shows that we do not have to do a complete calculation of all $\zeta(l)$ terms, since $\widetilde{Z}(n,l)$ is automatically zero if $rn \geqslant (r+s)(l-1) - t$. It also shows the tremendous cancellations which must take place within each $\zeta(l)$ coefficient.

For the n-bubble diagram, we see how delicate cancellations among the $\zeta(l)$ terms plus the $R(n)$ term must be (remember $|\widetilde{Z}(n,n+1)| \gg a_n$). For instance, for $n = 13$, we have $a_n \sim 10^{-2}$, while $|\widetilde{Z}(n,n+1)| \sim 10^5$! From the tables one notices the sign of $\widetilde{Z}(n,n)$, $\widetilde{Z}(n,n-1)$, and $R(n)$ is $(-1)^{n-1}$ and that is just the opposite sign of $\widetilde{Z}(n,n+1)$. One also notices for a given n that $|\widetilde{Z}(n,l)|$ becomes smaller for decreasing l and that the last which differs from zero is very small (compared to $|\widetilde{Z}(n,n+1)|$). We have no explanation for this behavior.

III. TWO EXAMPLES

Before we go on with the proof of the theorem [see Eq. (36), Sec. IV] we will consider two simple illustrative examples, one of which having $r = 1$ and the other one having $r = 0$. They both have the advantage that the rule Eq. (23), in these specific cases, can be seen clearly and in a very explicit way.

As our first example (I), we choose $f(x)$ to be of the form

$$f_{\rm I}(x) = -1 - \frac{\log(1-x)}{x}. \qquad (25)$$

Clearly we have $r = s = 1$, so following the general rule Eq. (23), $\widetilde{Z}_{\rm I}(n,l)$ should vanish for $n \geqslant 2l - 2 - t$. As usual $\widetilde{Z}_{\rm I}(n,l)$ is defined through the integral

$$a_n = \int_0^1 dx\, x^t [f_{\rm I}(x)]^n \qquad (26)$$

$$= \sum_{l=2}^{n+1} \zeta(l) \widetilde{Z}_{\rm I}(n,l) + R(n). \qquad (27)$$

Using Eq. (C17), we find easily

$$\widetilde{Z}_{\rm I}(n,l) = \frac{n!}{(n-1-t)!} \times \sum_{i=0}^{n+1-l} (-1)^i \binom{n-1-t}{i} \begin{bmatrix} n+1-l-i \\ n-1-t-i \end{bmatrix}. \qquad (28)$$

Introducing the notation $N \equiv n - 1 - t - i$ and $M \equiv l - 2 - t$ and using the following expansion theorem,[9]

$$\begin{bmatrix} N-M \\ N \end{bmatrix} = \sum_{\nu=0}^{M-1} |C_{M,\nu}| \binom{N}{2M-\nu}, \qquad (29)$$

where the numbers $|C_{M,\nu}|$ are nonnegative integers obeying the recursion relation

$$|C_{M+1,\nu}| = (2M + 1 - \nu)\{|C_{M,\nu}| + |C_{M,\nu-1}|\},$$

with

$$|C_{0,0}| \equiv 1,$$

$$|C_{M,\nu}| = 0 \quad \text{if } \nu > M - 1, \qquad (30)$$

and

$$|C_{M,\nu}| = 0 \quad \text{if } \nu < 0,$$

Eq. (28) becomes

$$\widetilde{Z}_{\rm I}(n,l) = \frac{n!}{(n-1-t)!} \sum_{i=0}^{n+1-l} (-1)^i \binom{n-1-t}{i} \begin{bmatrix} N-M \\ N \end{bmatrix}$$

$$= \frac{n!}{(n-1-t)!} \sum_{\nu=0}^{M-1} |C_{M,\nu}| \sum_{i=0}^{n-1-t} (-1)^i \binom{n-1-t}{i} \times \binom{n-1-t-i}{2l-4-2t-\nu} \qquad (31)$$

(notice that the i sum stops at $n - 1 - t$). Finally, using[9]

$$\sum_{i=0}^{r} (-1)^i \binom{r}{i} \binom{r-i}{m} = \delta_{r,m}, \qquad (32)$$

Eq. (31) becomes

$$\widetilde{Z}_{\rm I}(n,l) = \frac{n!}{(n-1-t)!} |C_{l-2-t,\,2l-3-t-n}|. \qquad (33)$$

Using Eqs. (30) and (33), we find $\widetilde{Z}_{\rm I}(n,l) = 0$ if $n \geqslant 2l - 2 - t$ which is exactly the result expected. In Table V, we have shown $\widetilde{Z}_{\rm I}(n,l)$ for $n \leqslant 9$, for the case $t = 0$. This example has also the asymptotic behavior $a_n \sim n!$ (obtained by letting $x \to 1$ and using the method of steepest descents), like a_n for the n-bubble diagram. Example I, therefore, displays all the features of the n-bubble diagram.

As our second example (II) we take

$$f_{\rm II}(x) = -\frac{1}{x} - \frac{1}{x^2} \log(1-x). \qquad (34)$$

Clearly $s = 2$ and $r = 0$ so that in this case our theorem tells us that $\widetilde{Z}_{\rm II}(n,l) = 0$ if $t \geqslant 2l - 2$ for all n (i.e., our condition becomes independent of n). Following steps similar to those which led to Eq. (33) we find

$$\widetilde{Z}_{\rm II}(n,l) = \frac{n!}{(2n-1-t)!} |C_{n+l-2-t,\,2l-3-t}|. \qquad (35)$$

From Eq. (30) and (35) it follows that $\widetilde{Z}(n,l) = 0$, if $t \geqslant 2l - 2$ for all n, as expected. In Table VI we have shown $\widetilde{Z}_{\rm II}(n,l)$, for $n \leqslant 9$, in the case $t = 7$.

TABLE V. $\widetilde{Z}_I(n,l)$, the coefficient of $\zeta(l)$ in a_n for example I. [see Eq. (33)].

$n \backslash l$	2	3	4	5	6	7	8	9	10
1	1								
2	0	0							
3	0	3	0						
4	0	0	8	0					
5	0	0	15	30	0				
6	0	0	0	120	144	0			
7	0	0	0	105	910	840	0		
8	0	0	0	0	1680	7392	5760	0	
9	0	0	0	0	945	2142	65772	45360	0

TABLE VI. $\widetilde{Z}_{\rm II}(n,l)$, the coefficient $\zeta(l)$ in a_n for example II. [see Eq. (35)].

$n \backslash l$	2	3	4	5	6	7	8	9	10
1	0								
2	0	0							
3	0	0	0						
4	0	0	0	24					
5	0	0	0	60	0				
6	0	0	0	90	180	0			
7	0	0	0	105	910	840	0		
8	0	0	0	105	2380	7308	5040	0	
9	0	0	0	181/2	4410	30366	31688/5	36288	0

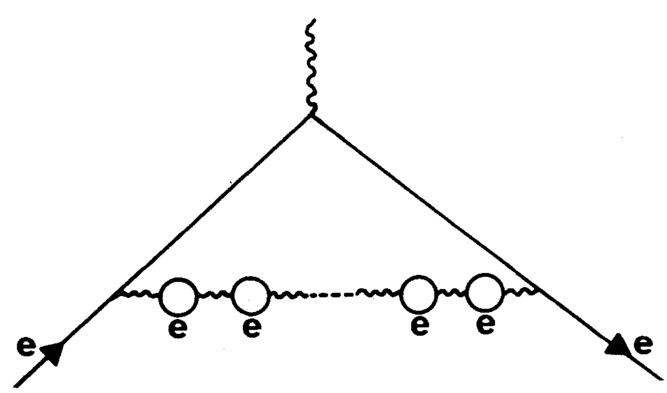

FIG. 1. The mass-independent n-bubble diagram contributing to g-2 of the electron.

IV. PROOF OF THEOREM

In this chapter we shall prove the theorem stated in Eq. (23). We shall repeat it here. Let $f(x)$ be a function of the form

$$f(x) = P(x) + Q(x)\log(1 - x), \tag{36}$$

with

$$P(x) = \sum_{i=0}^{s-1} \frac{p_i}{x^i},$$
$$Q(x) = \sum_{i=0}^{s} \frac{p_i}{x^i}, \quad s = 1,2,\cdots,$$

p_i, q_i being rational numbers. Furthermore, let $f(x) \to x^r$, $r = 0,1,2,\cdots$, as $x \to 0$. This last statement is satisfied [see Eqs. (B6) and (B7)] if

$$p_i = \sum_{k=1}^{s-i} \frac{q_{i+k}}{k}, \quad i = 0,1,\dots,s-1,$$

and

$$\frac{q_0}{i} = -\sum_{k=1}^{s} \frac{q_k}{i+k}, \quad i = 1,\dots,r-1. \tag{37}$$

Then, the $\zeta(l)$ coefficient in the integral

$$\int_0^1 dx\, x^t\, [f(x)]^n,$$

vanishes, whenever

$$rn \geqslant (r+s)(l-1) - t. \tag{38}$$

In the case $r = 0$, Eq. (38) says that the $\zeta(l)$ coefficient vanishes for all n, whenever

$$t \geqslant s(l-1). \tag{39}$$

Unlike the two examples in the previous section, we cannot prove the theorem in general in the explicit way we did it for the two examples. Instead we set up another appropriate finite integral, from which we will use the identities $D'(n,k) = 0$, $k = 0,1,\cdots$, $D'(n,k)$ being the coefficient of the divergence $\epsilon^{-k}(\epsilon^0 \equiv -\log\epsilon)$.

By choosing k carefully these identities can be brought into the form $Z'(n,l) = 0$, if Eq. (38) is satisfied. The trick is then to define

$$Z''(n,l) \equiv \widetilde{Z}(n,l) - Z'(n,l), \tag{40}$$

and show $Z''(n,l) = 0$, if Eq. (38) is satisfied. Then it follows easily that $\widetilde{Z}(n,l) = 0$, provided Eq. (38) is satisfied. The coefficient $\widetilde{Z}(n,l)$ is [see Eq. (C18)]

$$\widetilde{Z}(n,l) = (-q_s)^n\, n! \sum_{i=0}^{n+1-l} \frac{(-1)^i}{i!} \hat{\sum_1}(i) \times \sum_{j_1=0}^{n-i} \binom{n-i}{j_1} \left(\frac{q_{s-1}}{q_s}\right)^{j_1} \hat{\sum_2}(j_1) S(M,s,t), \tag{41}$$

with

$$m \equiv ns - 1 - t - p - q - i,$$

$$p \equiv \sum_{k=1}^{s-1} i_k,$$

and

$$q \equiv \sum_{k=1}^{s} j_k.$$

The "operators" $\hat{\Sigma}_{1,2}$ are defined in Eq. (C17) and repeated here,

$$\hat{\sum_1}(i) \equiv \sum \binom{i}{i_1} \cdots \binom{i_{s-2}}{i_{s-1}} \left(\frac{p_0}{p_1}\right)^{i_{s-1}} \cdots \left(\frac{p_{s-2}}{p_{s-1}}\right)^{i_1},$$

and

$$\hat{\sum_2}(j_1) \equiv \sum \binom{j_1}{j_2} \cdots \binom{j_{s-1}}{j_s} \left(\frac{q_0}{q_1}\right)^{j_s} \cdots \left(\frac{q_{s-2}}{q_{s-1}}\right)^{j_2}, \tag{42}$$

with the requirement that everything following $\hat{\Sigma}_{1,2}$ depending on the i_k's or j_k's are to be included in the sum. The limits in the sums $\hat{\Sigma}_1$, $\hat{\Sigma}_2$ are given by $0 \leqslant i_{s-1} \leqslant \cdots \leqslant i_1 \leqslant i$ and $0 \leqslant j_s \leqslant \cdots \leqslant j_1$, respectively. We have also used the compact notation($M \equiv p + q$),

$$S(M,s,t) \equiv \frac{1}{(n\cdot s - 1 - t - M - i)!} \begin{bmatrix} n+1-l-i \\ ns - 1 - t - M - i \end{bmatrix}. \tag{43}$$

The i-, l-, and n-dependence are omitted since they play no essential role in the proof. Clearly from Eq. (43) we have

$$S(M+1,s,t) = S(M,s,t+1). \tag{44}$$

Next, we define $g(x) \equiv f(x)/x^r$ which is well behaved at $x = 0$, since $f(x) \to x^r$. Now from Eqs. (C20) and (C21) it follows that the coefficient $D'(n,k)$ of ϵ^{-k}, in the (finite) integral

$$\int_0^1 dx [\, g(x)]^{n+1-l},$$

is

$$D'(n,k) = (-q_s)^n\, n! \sum_{i=0}^{n+1-l} \frac{(-1)^i}{i!} \hat{\sum_1}(i) \times \sum_{j_1=0}^{n+1-l-i} \binom{n+1-l-i}{j_1} \left(\frac{q_{s-1}}{q_s}\right)^{j_1} \hat{\sum_2}(j_1) \times \frac{1}{m'!} \begin{bmatrix} n+1-l-i \\ m' \end{bmatrix}, \tag{45}$$

with $m' \equiv (n+1-l)(r+s) - 1 - M - i - k$ and $D'(n,k) = 0$ for all $k = 0,1,2,\dots$ By letting $k \equiv rn - (r+s)(l-1) + t$, we have, for all n satisfying

$$rn \geqslant (r+s)(l-1) - t,$$

that $Z'(n,l) \equiv D'(n,k) = 0$. Now, with

$$D'(n,k) = (-q_s)^n\, n! \sum_{i=0}^{n+1-l} \frac{(-1)^i}{i!} \hat{\sum_1}(i) \times \sum_{j_1=0}^{n+1-l-i} \binom{n+1-l-i}{j_1} \times \left(\frac{q_{s-1}}{q_s}\right)^{j_1} \hat{\sum_2}(j_1)\, S(M,s,t), \tag{46}$$

these are the needed identities.

We shall first prove the theorem in the case of $f(x)$ coming from the n-bubble diagram. In this case $r = 2$, $s = 3$, and Eqs. (41) and (46) read

$$\widetilde{Z}(n,l) = (-q_3)^n\, n! \sum_{i=0}^{n+1-l} (-1)^i \hat{\sum_1}(i)$$

$$\times \sum_{j_1=0}^{n-i} \binom{n-i}{j_1} \left(\frac{q_2}{q_3}\right)^{j_1} \hat{\sum_2} (j_1) S(M,3,t), \quad (47)$$

and

$$Z'(n,l) = (-q_3)^n n! \sum_{i=0}^{n+1-l} \frac{(-1)^i}{i!} \hat{\sum_1} (i) \times \sum_{j_1=0}^{n+1-l-i} \binom{n+1-l-i}{j_1} \times \left(\frac{q_2}{q_3}\right)^{j_1} \hat{\sum_2} (j_1) S(M,3,t), \quad (48)$$

with $Z'(n,l) = 0$ if $2n \geqslant 5(l-1) - t$, $t = 0,1,2,\cdots$.

The j_1 sum can be extended up to $j_1 = n-i$ and, using the identity

$$\binom{n-i}{j_1} - \binom{n+1-l-i}{j_1} = \sum_{k=0}^{l-2} \binom{n+1-l-i+k}{j_1-1}, \quad (49)$$

we find, for the difference,

$$Z''(n,l) \equiv \tilde{Z}(n,l) - Z'(n,l) = (-q_3)^n n! \sum_{k=0}^{l-2} \sum_{i=0}^{n+1-l} \frac{(-1)^i}{i!} \hat{\sum_1} (i) \times \sum_{j_1=1}^{n+2-l-i+k} \binom{n+1-l-i+k}{j_1-1} \times \left(\frac{q_2}{q_3}\right)^{j_1} \hat{\sum_2} (j_1) S(M,3,t). \quad (50)$$

After changing $j_1 \to j_1 + 1$, Eq. (50) becomes

$$\frac{q_2}{q_3} (-q_3)^n n! \sum_{k=0}^{l-2} \sum_{i=0}^{n+1-l} \frac{(-1)^i}{i!} \hat{\sum_1} (i) \times \sum_{j_1=0}^{n+1-l-i+k} \binom{n+1-l-i+k}{j_1} \left(\frac{q_2}{q_3}\right)^{j_1} \hat{\sum_2} (j_1+1) \times S(M,3,t+1). \quad (51)$$

Using the identity

$$\binom{j_1+1}{j_2} = \binom{j_1}{j_2-1} + \binom{j_1}{j_2}, \quad (52)$$

we find

$$\hat{\sum_2} (j_1+1) S(M,3,t+1) = \sum_{j_2=0}^{j_1+1} \binom{j_1+1}{j_2} \left(\frac{q_0}{q_2}\right)^{j_2} S(M,3,t+1) = \sum_{j_2=1}^{j_1+l} \binom{j_1}{j_2-1} \left(\frac{q_0}{q_2}\right)^{j_2} S(M,3,t+1) + \sum_{j_2=0}^{j_1} \binom{j_1}{j_2} \left(\frac{q_0}{q_2}\right)^{j_2} S(M,3,t+1) = \frac{q_0}{q_2} \hat{\sum_2} (j_1) S(M,3,t+3) + \hat{\sum_2} (j_1) S(M,3,t+1), \quad (53)$$

where the last equality is obtained by changing $j_2 \to j_2 + 1$ in the first sum. Using Eqs. (51) and (53), we find

$$Z''(n,l) = (-q_3)^n n! \sum_{k=0}^{l-2} \sum_{i=0}^{n+1-l} \frac{(-1)^i}{i!} \hat{\sum_1} (i) \times \sum_{j_1=0}^{n+1-l-i+k} \binom{n+1-l-i+k}{j_1} \times \left(\frac{q_2}{q_3}\right)^{j_1} \hat{\sum_2} (j_1) \times \left\{ \frac{q_2}{q_3} S(M,3,t+1) + \frac{q_0}{q_3} S(M,3,t+3) \right\}. \quad (54)$$

Clearly, it is sufficient to show that the term containing $S(M,3,t+1)$ is zero, since the other term is obtained from this by changing $t \to t+2$. We will now show that each term in the k-sum is zero. This is done by mathematical induction in k. First for $k=0$ Eq. (54) (second term omitted) becomes

$$Z''(n,l) = (-q_3)^n \left(\frac{q_2}{q_3}\right) n! \sum_{i=0}^{n+1-l} \frac{(-1)^i}{i!} \hat{\sum_1} (i) \times \sum_{j_1=0}^{n+1-l-i} \binom{n+1-l-i}{j_1} \left(\frac{q_2}{q_3}\right)^{j_1} \times \hat{\sum_2} (j_1) S(M,3,t+1), \quad (55)$$

which is nothing but $q_2/q_3 [Z'(n,l)|_{t \to t+1}]$ [see Eq. (48)]. Now, from Eq. (48), $Z'(n,l) = 0$ if $2n \geqslant 5(l-1) - 1 - t$, and clearly this is also true under the weaker condition $2n \geqslant 5(l-1) - t$. Therefore, we also have $\tilde{Z}''(n,l) = 0$ if $2n \geqslant 5(l-1) - t$. This is what we wanted. Suppose that the k term denoted by $Z''(n,l,k)$ is zero for $2n \geqslant 5(l-1) - t$. Then we must show $Z''(n,l,k+1) = 0$.

Using

$$Z''(n,l,k) = (-q_3)^n \left(\frac{q_2}{q3}\right) n! \sum_{i=0}^{n+1-l} \frac{(-1)^i}{i!} \hat{\sum_1} (i) \times \sum_{j_1=0}^{n+1-l-i+k} \binom{n+1-l-i+k}{j_1} \left(\frac{q_2}{q3}\right)^{j_1} \times \hat{\sum_2} (j_1) S(M,3,t+1) \quad (56)$$

(and following steps similar to those used above), we find

$$Z''(n,l,k+1) - Z''(n,l,k) = (-q_3)^n \left(\frac{q_2}{q_3}\right) n! \sum_{i=0}^{n+1-l} \frac{(-1)^i}{i!} \hat{\sum_1} (i) \times \sum_{j_1=0}^{n+1-l-i+k} \binom{n+1-l-i+k}{j_1} \left(\frac{q_2}{q_3}\right)^{j_1} \hat{\sum_2} (j_1) \times \left\{ \frac{q_2}{q_3} S(M,3,t+2) + \frac{q_0}{q_3} S(M,3,t+4) \right\}, \quad (57)$$

which is nothing but

$$\left(\frac{q_2}{q_3}\right) Z''(n,l,k) \Big|_{t \to t+1} + \left(\frac{q_0}{q_3}\right) Z''(n,l,k) \Big|_{t \to t+3}. \quad (58)$$

Using the induction assumption, $Z''(n,l,k) = 0$, Eq. (58) implies that $Z''(n,l,k+1) = 0$. This ends the induction proof.

Now, in the general case, we have a string of binomial coefficients,

$$\binom{j_1}{j_2} \binom{j_2}{j_3} \cdots \binom{j_{s-1}}{j_s}, \quad (59)$$

which can be expanded as

$$\binom{j_1-1}{j_2-1}\cdots\binom{j_{s-2}-1}{j_{s-1}-1}\binom{j_{s-1}-1}{j_s-1} + \binom{j_1-1}{j_2-1}\cdots\binom{j_{s-2}-1}{j_{s-1}-1}\binom{j_{s-1}-1}{j_s} + \cdots + \binom{j_1-1}{j_2}\cdots\binom{j_{s-1}}{j_s}. \tag{60}$$

Following the same steps as before, we find from Eq. (60) that

$$Z''(n,l) = (-q_s)^n\, n! \sum_{k=0}^{l-2} \frac{(-1)^i}{i!} \sum_{i=0}^{n+1-l} \hat{\sum_1}(i) \times \sum_{j_1=0}^{n+1-l-i+k} \binom{n+1-l-i+k}{j_1} \left(\frac{q_{s-1}}{q_s}\right)^{j_1} \times \hat{\sum_2}(i) \sum_{k'=0}^{s-1} \frac{q_{k'}}{q_s} S(M,s,t+s-k'). \tag{61}$$

Again, looking at the term with $k'=s-1$ is sufficient to prove $Z''(n,l)=0$, now for $rn \geqslant (r+s)(l-1)-t$. This now follows easily by using the same techniques which led to Eq. (58). This completes the proof in the general case.

Up to now our functions $f(x)$ did not have any positive powers of x in them. We shall see below that the theorem also works nicely in that case. Before we do this in general, we take a simple example. Let

$$f(x) = \frac{x}{2} + 1 + \frac{\log(1-x)}{x}. \tag{62}$$

Clearly $s=1, r=2$ so that $\widetilde{Z}(n,l)=0$, if $2n \geqslant 3(l-1)-t$. [If the rule Eq. (38) is correct.] Define

$$g(x) = \frac{f(x)}{x} = \frac{1}{2} + \frac{1}{x} + \frac{\log(1-x)}{x^2}, \tag{63}$$

where $g(x)$ now is of the usual form [see Eq. (38)] with $s=2$, $r=1$. Now

$$\int_0^1 dx\, x^t [f(x)]^n = \int_0^1 dx\, x^{n+t} [g(x)]^n, \tag{64}$$

from which follows $\widetilde{Z}(n,l)=0$ if $n \geqslant 3(l-1)-(n+t)$ or $2n \geqslant 3(l-1)-t$, exactly as expected. Now we take the general theorem. Let again

$$f(x) = P(x) + Q(x)\log(1-x),$$

but now with

$$P(x) = \sum_{k=-m}^{s'-1} \frac{p_k}{x^k},$$

$$Q(x) = \sum_{k=-m}^{s'} \frac{q_k}{x^k}, \quad m=0,1,2,\cdots, \tag{65}$$

and such that $f(x) \underset{x\to 0}{\longrightarrow} x^{r'}$, $r'=0,1,2,\cdots$, then $\widetilde{Z}(n,l)=0$ if $nr' \geqslant (r'+s')(l-1)-t'$. $\widetilde{Z}(n,l)$ is being defined through the integral

$$\int_0^1 dx\, x^{t'} [f(x)]^n. \tag{66}$$

Since we must have $m \leqslant r'$, we can define

$$g(x) = f(x)/x^m,$$

and $g(x)$ is now a function of the usual form with $s=s'+m$ and $r=r'-m$. Then Eq. (66) reads

$$\int_0^1 dx x^{t'} [f(x)]^n = \int_0^1 dx\, x^t [g(x)]^n, \tag{67}$$

with $t=t'+nm$. The theorem used in Eq. (38) gives $\widetilde{Z}(n,l)=0$ if

$$rn \geqslant (r+s)(l-1)-t = (r'-m+s'+m)(l-1)-t'-nm, \quad \text{or}$$

$$nr \geqslant (r'+s')(l-1)-t'. \tag{68}$$

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APPENDIX A

We shall derive the exact expression for the integral

$$I_\epsilon(n,m) = \int_\epsilon^1 \frac{\log^n(1-x)}{x^{m+1}} dx, \quad n,m=0,1,2,\cdots, \tag{A1}$$

where we are interested in the limit $\epsilon \to 0$. $I_\epsilon(n,m)$ is a sum of a divergent part $D_\epsilon(n,m)$, a finite term $Z(n,m)$ consisting of Riemann zeta functions with rational coefficients, and a finite rational term $R(n,m)$.

$$I_\epsilon(n,m) = D_\epsilon(n,m) + Z(n,m) + R(n,m). \tag{A2}$$

Let us first find $D_\epsilon(n,m)$. We shall use the fact that $\log^n(1-x)$ is the generating function of the Stirling numbers of the first kind,[9]

$$\log^n(1-x) = (-1)^n\, n! \sum_{k=n}^{\infty} \frac{1}{k!} \begin{bmatrix} n \\ k \end{bmatrix} x^k, \tag{A3}$$

where we define $\left[{n \atop k}\right] \equiv |S_k^{(n)}|$, $S_k^{(n)}$ being the Stirling numbers of the first kind. The numbers $\left[{n \atop k}\right]$ are nonnegative integers which obey the recursion relation

$$\begin{bmatrix} n \\ k+1 \end{bmatrix} = \begin{bmatrix} n-1 \\ k \end{bmatrix} + k \begin{bmatrix} n \\ k \end{bmatrix}, \tag{A4}$$

with

$$\begin{bmatrix} n \\ k \end{bmatrix} = 0, \quad \text{if } k < n,$$

and

$$\begin{bmatrix} n \\ n \end{bmatrix} = 1.$$

Using Eqs. (A1) and (A3), we obtain

$$I_\epsilon(n,m) = (-1) \sum_{k=n}^{\infty} \frac{1}{k!} \begin{bmatrix} n \\ k \end{bmatrix} \int_\epsilon^1 \frac{dx}{x^{m+1-k}}. \tag{A5}$$

The divergent terms in Eq. (A5) come from $k=n,\ldots,m$ only. Thus

$$D_\epsilon(n,m) = (-1)^n\, n! \sum_{k=n}^{m} \frac{1}{k} \begin{bmatrix} n \\ k \end{bmatrix} \int_\epsilon^1 \frac{dx}{x^{m+1-k}} = (-1)^n\, n! \left\{ \frac{1}{m!} \begin{bmatrix} n \\ m \end{bmatrix} (-\log\epsilon) + \sum_{k=n}^{m-1} \frac{1}{k!} \right.$$

$$\times \begin{bmatrix} n \\ k \end{bmatrix} \frac{1}{m-k} \frac{1}{\epsilon^{m-k}} \Big\}, \tag{A6}$$

or, changing $k \to m - k$ in Eq. (A6),

$$D_\epsilon(n,m) = (-1)^n n! \left\{ \frac{1}{m!} \begin{bmatrix} n \\ m \end{bmatrix} (-\log \epsilon) + \sum_{k=1}^{m-n} \frac{1}{k} \cdot \frac{1}{(m-k)!} \begin{bmatrix} n \\ m-k \end{bmatrix} \frac{1}{\epsilon^k} \right\}. \tag{A7}$$

All $O(1)$ terms have been omitted in Eqs. (A6) and (A7). We now go on to the finite parts of $I_\epsilon(n,m)$. First let $m = 0$, for $n \geqslant 1$. Then Eq. (A1) becomes

$$I_\epsilon(n,0) = \int_\epsilon^1 \frac{\log^n(1-x)}{x} dx = (-1)^n n! \zeta(n+1). \tag{A8}$$

From Eqs. (A2) and (A8) we obtain

$$Z(n,0) = (-1)^n n! \zeta(n+1)$$

and

$$R(n,0) = 0. \tag{A9}$$

If $m,n \geqslant 1$, we can instead perform a partial integration on x^{-m-1}:

$$\begin{aligned} I_\epsilon(n,m) &= \int_\epsilon^1 dx \cdot \frac{\log^n(1-x)}{x^{m+1}} \\ &= \frac{1}{m} \frac{\log^n(1-x)}{x^m}\Big|_\epsilon^1 \\ &\quad - \frac{n}{m} \int_\epsilon^1 dx \frac{\log^{n-1}(1-x)}{(1-x)x^m}. \end{aligned} \tag{A10}$$

Using the identity (easily proved by induction after m)

$$\frac{1}{1-x} \frac{1}{x^m} = \frac{1}{1-x} + \frac{1}{x} + \sum_{i_1=1}^{m-1} \frac{1}{x^{i_1+1}},$$

Eq. (A10) becomes

$$\begin{aligned} I_\epsilon(n,m) &= \frac{1}{m} \log^n(1-x) \left[\frac{1}{x^m} - 1 \right]_\epsilon^1 \\ &\quad - \frac{n}{m} \int_0^1 dx \frac{\log^{n-1}(1-x)}{x} \\ &\quad - \frac{n}{m} \sum_{i_1=1}^{m-1} \int_\epsilon^1 dx \frac{\log^{n-1}(1-x)}{x^{i_1+1}} \\ &= \frac{1}{m} \frac{\log^{n-1}(1-\epsilon)}{\epsilon^m} + (-1)^n \frac{n!}{m} \zeta(n) \\ &\quad - \frac{n}{m} \sum_{i_1=1}^{m-1} I_\epsilon(n-1, i_1). \end{aligned} \tag{A11}$$

Finally, using Eqs. (A3) and (A11), we obtain

$$\begin{aligned} I_\epsilon(n,m) &= (-1)^n \frac{n!}{m} \sum_{k=n}^{m-1} \frac{1}{k!} \begin{bmatrix} n \\ k \end{bmatrix} \frac{1}{\epsilon^{m-k}} \\ &\quad + (-1)^n \frac{n!}{mm!} \begin{bmatrix} n \\ m \end{bmatrix} + (-1)^n \frac{n!}{m} \zeta(n) \\ &\quad - \frac{n}{m} \sum_{i_1=1}^{m-1} I_\epsilon(n-1, i_1). \end{aligned} \tag{A12}$$

From Eqs. (A2) and (A12) we read off the two recursion relations

$$Z(n,m) = (-1)^n \frac{n!}{m} \zeta(n) - \frac{n}{m} \sum_{i_1=1}^{m-1} Z(n-1, i_1) \tag{A13}$$

and

$$R(n,m) = (-1)^n \frac{n!}{mm!} \begin{bmatrix} n \\ m \end{bmatrix} - \frac{n}{m} \sum_{i_1=1}^{m-1} R(n-1, i_1), \tag{A14}$$

with

$$\begin{aligned} R(1,m) &= \frac{1}{m^2} + \frac{1}{m} \sum_{i_1=1}^{m-1} \frac{1}{i_1} \\ &= -\frac{1}{m^2} + \frac{1}{m!} \begin{bmatrix} 2 \\ m \end{bmatrix}. \end{aligned}$$

We shall first concentrate on the $Z(n,m)$ part. Using Eq. (A13) recursively $n-2$ times gives

$$\begin{aligned} Z(n,m) &= (-1)^n \frac{n!}{m} \zeta(n) + (-1)^n \frac{n!}{m} \sum_{k=2}^{n-1} \\ &\quad \times \zeta(n+1-k) \sum_{i_1=1}^{m-1} \frac{1}{i_1} \cdots \sum_{i_{k-1}=1}^{i_{k-2}-1} \frac{1}{i_{k-1}}. \end{aligned} \tag{A15}$$

Equation (A15) can be written in a more compact way, by making use of the definition of the Stirling numbers of the first kind. We have simply

$$\begin{bmatrix} k \\ m \end{bmatrix} = (m-1)! \sum_{i_1=1}^{m-1} \frac{1}{i_1} \cdots \sum_{i_{k-1}=1}^{i_{k-2}-1} \frac{1}{i_{k-1}}. \tag{A16}$$

Using the definition of $\left[{k \atop m}\right]$ given in Eq. (A16), we have

$$Z(n,m) = (-1)^n \frac{n!}{m} \sum_{k=2}^{n-1} \zeta(n+1-k) \begin{bmatrix} k \\ m \end{bmatrix}. \tag{A17}$$

Finally, using Eq. (A9) together with $\left[{0 \atop m}\right] = \delta_{0,m}$ and $\left[{1 \atop m}\right] = (m-1)!$, we have, for all $m = 0,1,2,\cdots$,

$$Z(n,m) = (-1)^n \frac{n!}{m!} \times \sum_{k=0}^{n-1} \zeta(n+1-k) \begin{bmatrix} k \\ m \end{bmatrix}. \tag{A18}$$

Now we move on to the rational term $R(n,m)$. Since $\left[{n \atop m}\right] = 0$, if $m < n$, we read off from Eq. (A14) that

$$R(n,m) = 0, \quad \text{if } m < n,$$

while for the diagonal term $R(n,n)$ we have

$$R(n,n) = \frac{(-1)^n}{n} - R(n-1, n-1).$$

Repeated use of this equation gives

$$\begin{aligned} R(n,n) &= (-1)^n \sum_{i=1}^{n} \frac{1}{i} \\ &= \frac{(-1)^n}{n!} \begin{bmatrix} 2 \\ n+1 \end{bmatrix}. \end{aligned} \tag{A19}$$

A recursion relation, like the one we have for $\left[{n \atop m}\right]$, can be obtained from Eq. (A14) by letting $m \to m+1$:

$$\begin{aligned} R(n,m+1) &= \frac{(-1)^n n!}{(m+1)(m+1)!} \begin{bmatrix} n \\ m+1 \end{bmatrix} - \frac{n}{m+1} \\ &\quad \times \sum_{i_1=0}^{m} R(n-1, i_1) \\ &= \frac{(-1)^n n!}{(m+1)(m+1)!} \begin{bmatrix} n-1 \\ m \end{bmatrix} \end{aligned}$$

$$+\frac{(-1)^n n!m}{(m+1)(m+1)!}\begin{bmatrix} n \\ m \end{bmatrix} - \frac{n}{m+1} R(n-1,m)$$

$$-\frac{n}{m+1}\sum_{i_1=0}^{m-1} R(n-1,i_1)$$

$$=\frac{m}{m+1} R(n,m) - \frac{n}{m+1} R(n-1,m)$$

$$+\frac{(-1)^n n!}{(m+1)(m+1)!}\left\{\begin{bmatrix} n-1 \\ m \end{bmatrix} - \begin{bmatrix} n \\ m \end{bmatrix}\right\}. \tag{A20}$$

We could have stopped here, since Eqs. (A19) and (A20) would be sufficient to calculate $R(n,m)$. However, we have written $R(n,m)$ in the alternative way,

$$R(n,m) = (-1)^{n+1}\frac{n!}{m!}\begin{bmatrix} n+1 \\ m \end{bmatrix} + (-1)^n \frac{n!}{(m!)^2}\left[\begin{bmatrix} n \\ m \end{bmatrix}\right]. \tag{A21}$$

The numbers $[[{n \atop m}]]$ are, like $[{n \atop m}]$, nonnegative integers, and obey the recursion relation

$$\left[\begin{bmatrix} n \\ m+1 \end{bmatrix}\right] = m(m+1)\left[\begin{bmatrix} n \\ m \end{bmatrix}\right] + (m+1)\left[\begin{bmatrix} n-1 \\ m \end{bmatrix}\right]$$

$$+ m\begin{bmatrix} 1 \\ m \end{bmatrix}\left\{\begin{bmatrix} n-1 \\ m \end{bmatrix} - \begin{bmatrix} n \\ m \end{bmatrix}\right\},$$

with

$$\left[\begin{bmatrix} n \\ m \end{bmatrix}\right] = 0 \quad \text{if } m < n,$$

$$\left[\begin{bmatrix} n \\ n \end{bmatrix}\right] = \begin{bmatrix} 2 \\ n+1 \end{bmatrix}, \tag{A22}$$

$$\left[\begin{bmatrix} 1 \\ m \end{bmatrix}\right] = \begin{bmatrix} 1 \\ m \end{bmatrix}^2.$$

All this follows easily from Eqs. (A19) and (A20).

The motivation for this, apart from an aesthetic one, is seen by using Eq. (A14) recursively $n-1$ times:

$$R(n,m) = (-1)^n \frac{n!}{m!}$$

$$\times\left\{\frac{1}{m!}\begin{bmatrix} n \\ m \end{bmatrix} + \sum_{i_1=1}^{m-1}\frac{1}{i_1 i_1!}\begin{bmatrix} n-1 \\ i_1 \end{bmatrix} + \cdots\right.$$

$$+\sum_{i_1=1}^{m-1}\frac{1}{i_1}\cdots\sum_{i_{n-1}=1}^{i_{n-2}-1}\frac{1}{i_{n-1}}\left[\frac{1}{i_{n-1}}\right.$$

$$\left.\left.+\sum_{i_n=1}^{i_{n-1}-1}\frac{1}{i_n}\right]\right\}$$

$$=(-1)^{n+1}\frac{n!}{m!}\begin{bmatrix} n+1 \\ m \end{bmatrix}$$

$$+(-1)^n\frac{n!}{(m!)^2}\left[\begin{bmatrix} n \\ m \end{bmatrix}\right], \tag{A23}$$

with

$$\left[\begin{bmatrix} n \\ m \end{bmatrix}\right] \equiv \begin{bmatrix} 1 \\ m \end{bmatrix}\begin{bmatrix} 1 \\ m+1 \end{bmatrix}$$

$$\times\left\{\frac{1}{m!}\begin{bmatrix} n \\ m \end{bmatrix} + \sum_{i_1=1}^{m-1}\frac{1}{i_1 i_1!}\begin{bmatrix} n-1 \\ i_1 \end{bmatrix} + \cdots\right.$$

$$\left.+\sum_{i_1=1}^{m-1}\frac{1}{i_1}\cdots\sum_{i_{n-1}=1}^{i_{n-2}-1}\frac{1}{i_{n-1}i_{n-1}!}\begin{bmatrix} 1 \\ i_{n-1} \end{bmatrix}\right\}.$$

One last and simple result is needed. For $m < 0$, one finds easily that

$$R(n,m) = (-1)^n n! \sum_{i=0}^{-1-m}(-1)^i\binom{-1-m}{i}$$

$$\times\frac{1}{(1+i)^{n+1}}. \tag{A24}$$

APPENDIX B

We shall consider functions $f(x)$ of the form:

$$f(x) = P(x) + Q(x)\cdot\log(1-x), \tag{B1}$$

with

$$P(x) = \sum_{i=0}^{s'}\frac{p_i}{x^i}, \tag{B2}$$

$$Q(x) = \sum_{i=0}^{s}\frac{q_i}{x^i},$$

$s', s = 0,1,2,\ldots$, and p_i, q_i being rational numbers. In the limit $x \to 0$, we demand $f(x)$ to be finite and to have a Taylor-series expansion, with the first $r-1$ coefficients vanishing:

$$f(x) \underset{x\to 0}{\to} C_{r-1}x^{r-1} + C_r x^r + \cdots. \tag{B3}$$

We will find the relationships among the p_i, q_i's such that Eq. (B3) is satisfied. By Taylor-series expansion of $\log(1-x)$,

$$\log(1-x) = -\sum_{k=1}^{\infty}\frac{x^k}{k},$$

Eq. (B1) becomes

$$f(x) = \sum_{i'=0}^{s'}\frac{p_{i'}}{x^{i'}} - \sum_{k=1}^{\infty}\frac{q_0}{k}x^k - \sum_{k=1}^{\infty}\sum_{i=1}^{s}\frac{q_i}{k}x^{k-1}$$

$$= \sum_{i'=0}^{s'}\frac{p_{i'}}{x^{i'}} - \sum_{i=1}^{s}\sum_{k=1}^{i}\frac{q_i}{k}x^{k-1}$$

$$-\sum_{k=1}^{\infty}\frac{q_0}{k}x^k - \sum_{i=1}^{s}\sum_{k=i+1}^{\infty}\frac{q_i}{k}x^{k-1}. \tag{B4}$$

For the second term in Eq. (B4), we change variables from i to $i' = i - k$, while for the fourth term we let $k \to k + i$. Equation (B4) then becomes

$$\sum_{i'=0}^{s'}\frac{p_{i'}}{x^{i'}} - \sum_{i'=0}^{s-1}\sum_{k=1}^{s-i'}\frac{q_{i'+k}}{k}\frac{1}{x^{i'}}$$

$$+\sum_{k=1}^{\infty}x^k\left[\frac{q_0}{k} + \sum_{i=1}^{s}\frac{q_i}{k+i}\right]$$

$$= \sum_{i'=1}^{s'}\frac{p_{i'}}{x^{i'}} - \sum_{i'=0}^{s-1}\sum_{k=1}^{s-i'}\frac{q_{i'+k}}{k}\cdot\frac{1}{x^{i'}} + \left[p_0 - \sum_{k=1}^{s}\frac{q_k}{k}\right]$$

$$+\sum_{k=1}^{\infty}x^k\left[\frac{q_0}{k} + \sum_{i=1}^{s}\frac{q_i}{k+i}\right]. \tag{B5}$$

Now in order for $f(x)$ to be finite, the following indentities must be satisfied:

$$s' = s - 1,$$

$$p_i = \sum_{k=1}^{s-i} \frac{q_{i+k}}{k}, \quad i = 1,2,\ldots,s-1, \tag{B6}$$

and in order for $f(x)$ to satisfy Eq. (B3) we must have

$$p_0 = \sum_{k=1}^{s} \frac{q_k}{k},$$

$$\frac{q_0}{i} = -\sum_{k=1}^{s} \frac{q_k}{k+i}, \quad \text{for } i = 1,\ldots,r-1. \tag{B7}$$

Equation (B7) is to be understood in the following way: if $r \geqslant 2$, then both conditions must be satisfied, if $r = 1$, only the first condition must be satisfied; and if $r = 0$, none of the conditions need to be satisfied.

APPENDIX C

Here we shall extract the coefficient $\widetilde{Z}(n,l)$ of the $\zeta(l)$ term, the rational term $R(n)$, and also the divergent part $D(n)$ for the general integral

$$\int_0^1 dx x^t [f(x)]^n, \quad t = 0,1,2,\cdots, \tag{C1}$$

with $f(x)$ being defined in Appendix B. First, we do a binomial expansion of

$$[f(x)]^n = [P(x) + Q(x)\log(1-x)]^n$$
$$= \sum_{i=0}^{n} \binom{n}{i} [P(x)]^i [Q(x)]^{n-i} \log^{n-i}(1-x). \tag{C2}$$

Next, we use a multinomial expansion of $[P(x)]^i$ in Eq. (C2):

$$[P(x)]^i = \left[\frac{p_{s-1}}{x^{s-1}} + \frac{p_{s-2}}{x^{s-2}} + \cdots + \frac{p_1}{x} + p_0\right]^i$$
$$= \sum \binom{i}{i_1}\binom{i_1}{i_2}\cdots\binom{i_{s-2}}{i_{s-1}}\left(\frac{p_{s-1}}{x^{s-1}}\right)^{i_{s-1}}$$
$$\times \left(\frac{p_{s-2}}{x^{s-2}}\right)^{i_{s-2}-i_{s-1}} \cdots (p_0)^{i-i_1} \tag{C3}$$
$$= \sum \binom{i}{i_1}\cdots\binom{i_{s-2}}{i_{s-1}}(p_0)^{i_1}\left(\frac{p_i}{p_0}\right)^{i_1}$$
$$\times \cdots \left(\frac{p_{s-1}}{p_{s-2}}\right)^{i_{s-1}} \cdot \frac{1}{x^p},$$

where the summation goes over $0 \leqslant i_{s-1} \leqslant \cdots \leqslant i_1 \leqslant i$ and $p = \Sigma_{k=2}^{s-1} k(i_{k-1} - i_k) + (s-1)i_{s-1} = \Sigma_{k=1}^{s-1} i_k$. A multinomial expansion of $[Q(x)]^{n-i}$ gives similarly

$$[Q(x)]^{n-1} = \left[\frac{q_s}{x^s} + \frac{q_{s-1}}{x^{s-1}} + \cdots + \frac{q_1}{x} + q\right]^{n-i}$$
$$= \sum \binom{n-1}{j_1}\binom{j_1}{j_2}\cdots\binom{j_{s-1}}{j_s}(q_0)^{n-i}\left(\frac{q_1}{q_0}\right)^{j_1}$$
$$\times \cdots \left(\frac{q_s}{q_{s-1}}\right)^{j_s} \frac{1}{x^q}, \tag{C4}$$

where the summation goes over $0 \leqslant j_s \leqslant \cdots \leqslant j_1 \leqslant n-i$ and $q = \Sigma_{k=1}^{s} j_k$.

In Eqs. (C3) and (C4) we have assumed all $p_k, q_k \neq 0$. If, say, $q_k = 0$, then we define $j_k \equiv j_{k+1}$ ($j_0 \equiv n-i$) and

$$\left(\frac{q_k}{q_{k-1}}\right)^{j_k}\left(\frac{q_{k+1}}{q_k}\right)^{j_{k+1}} \equiv \left(\frac{q_{k+1}}{q_{k-1}}\right)^{j_{k+1}}. \tag{C5}$$

Using Eqs. (C2)–(C4), Eq. (C1) becomes

$$(q_0)^n \sum_{i=0}^{n} \binom{n}{i}\left(\frac{p_0}{q_0}\right)^i \sum \binom{i}{i_1}\cdots\binom{i_{s-2}}{i_{s-1}}$$
$$\times \left(\frac{p_1}{p_0}\right)^{i_1}\cdots\left(\frac{p_{s-1}}{p_{s-2}}\right)^{i_{s-1}}$$
$$\times \sum \binom{n-i}{j_i}\cdots\binom{j_{s-1}}{j_s}\left(\frac{q_1}{q_0}\right)^{j_1}\cdots\left(\frac{q_s}{q_{s-1}}\right)^{j_s}$$
$$\times I_\epsilon(n-i,m), \tag{C6}$$

with $m = p + q - l - t$, and the integral

$$I_\epsilon(n,m) \equiv \int_\epsilon^1 dx \frac{\log^n(1-x)}{n^{m+1}} \quad \text{as } \epsilon \to 0.$$

Using Eqs. (A2), (A18), and (C6), the part containing Riemann zeta functions becomes

$$(-q_0)^n n! \sum_{i=0}^{n-1} \frac{1}{i!}\left(-\frac{p_0}{q_0}\right)^i \sum \binom{i}{i_1}\cdots\binom{i_{s-2}}{i_{s-1}}$$
$$\times \left(\frac{p_1}{p_0}\right)^{i_1}\cdots\left(\frac{p_{s-1}}{p_{s-2}}\right)^{i_{s-1}}$$
$$\times \sum \binom{n-i}{j_1}\cdots\binom{j_{s-1}}{j_s}\cdot\left(\frac{q_1}{q_0}\right)^{j_1}\cdots\left(\frac{q_s}{q_{s-1}}\right)^{j_s}$$
$$\times \frac{1}{m!}\sum_{k=0}^{n-1-i} \zeta(n+1-i-k)\begin{bmatrix} k \\ m \end{bmatrix}. \tag{C7}$$

To find a specific $\zeta(l)$ coefficient, we change $k \to l - i$ in the double sum:

$$\sum_{i=0}^{n-1}\sum_{k=0}^{n-1-i} \zeta(n+1-i-k)\begin{bmatrix} k \\ m \end{bmatrix}$$
$$= \sum_{i=0}^{n-1}\sum_{l=i}^{n-1} \zeta(n+1-l)\begin{bmatrix} l-i \\ m \end{bmatrix}. \tag{C8}$$

Interchanging the i,l sum, Eq. (C8) becomes

$$\sum_{l=0}^{n-1} \zeta(n+1-l)\sum_{i=0}^{l}\begin{bmatrix} l-i \\ m \end{bmatrix}$$
$$= \sum_{l=2}^{n+1} \zeta(l)\sum_{i=0}^{n+i-l}\begin{bmatrix} n+1-l-i \\ m \end{bmatrix}. \tag{C9}$$

Equation (C7) now yields $\Sigma_{l=2}^{n+1}\widetilde{Z}(n,l)\zeta(l)$, with

$$\widetilde{Z}(n,l) = (-q_0)^n n! \sum_{i=0}^{n+1-l} \frac{1}{i!}\left(-\frac{p_0}{q_0}\right)^i$$
$$\times \sum \binom{i}{i_1}\cdots\binom{i_{s-2}}{i_{s-1}}\left(\frac{p_1}{p_0}\right)^{i_1}\cdots\left(\frac{p_{s-1}}{p_{s-2}}\right)^{i_{s-1}}$$
$$\times \sum \binom{n-i}{j_i}\cdots\binom{j_{s-1}}{j_s}\left(\frac{q_1}{q_0}\right)^{j_1}$$
$$\times \cdots \left(\frac{q_s}{q_{s-1}}\right)^{j_s}\frac{1}{m!}\begin{bmatrix} n+1-l-i \\ m \end{bmatrix}. \tag{C10}$$

Using Eqs. (A2) and (C6), we obtain for the rational term,

$$R(n) = (q_0)^n \sum_{i=0}^{n}\binom{n}{i}\left(\frac{p_0}{q_0}\right)^i \sum \binom{i}{i_1}$$

$$\times \cdots \binom{i_{s-2}}{i_{s-1}} \left(\frac{p_1}{p_0}\right)^{i_1} \cdots \left(\frac{p_{s-1}}{p_{s-2}}\right)^{i_{s-1}}$$
$$\times \sum \binom{n-i}{j_1} \cdots \binom{j_{s-1}}{j_s} \left(\frac{q_1}{q_0}\right)^{j_1} \cdots \left(\frac{q_s}{q_{s-1}}\right)^{j_s}$$
$$\times R(n-i,m). \qquad \text{(C11)}$$

In the case of the n-bubble diagram, we have $(p_0, p_1, p_2) = (-5/3, -4, 4)$ and $(q_0, q_1, q_2, q_3) = (1,0,-6,4)$. Now, using Eq. (C5) (since $q_1 = 0$ we have $j_1 = j_2$), Eqs. (C10) and (C11) read

$$\tilde{Z}(n,l) = \left(-\frac{1}{3}\right)^n n! \sum \frac{1}{i!} \left(\frac{5}{3}\right)^i \binom{i}{i_1} \left(\frac{12}{5}\right)^{i_1}$$
$$\times \binom{i_1}{i_2} (-1)^{i_2} \binom{n-i}{i_3} (-6)^{i_3} \binom{i_3}{i_4} \left(-\frac{2}{3}\right)^{i_4}$$
$$\times \left\{ \frac{1}{(m-1)!} \begin{bmatrix} n+1-l-i \\ m-1 \end{bmatrix} - \frac{1}{(m-2)!} \begin{bmatrix} n+1-l-i \\ m-2 \end{bmatrix} \right\}, \qquad \text{(C12)}$$

with $m = i_1 + i_2 + 2i_3 + i_4$ and the summation going over $0 \leqslant i_2 \leqslant i_1 \leqslant i \leqslant n+1-l$ and $0 \leqslant i_4 \leqslant i_3 \leqslant n-i$.

$$R(n) = \left(\frac{1}{3}\right)^n \sum \frac{1}{i!} \left(\frac{5}{3}\right)^i \binom{i}{i_1} \left(\frac{12}{5}\right)^{i_1}$$
$$\times \binom{i_1}{i_2} (-1)^{i_2}$$
$$\times \binom{n-i}{i_3} (-6)^{i_3} \binom{i_3}{i_4} \left(-\frac{2}{3}\right)^{i_4}$$
$$\times \{R(n-i,m-1) - R(n-i,m-2)\}, \qquad \text{(C13)}$$

with m as in Eq. (C11), and the summation going over $0 \leqslant i_2 \leqslant i_1 \leqslant i \leqslant n$ and $0 \leqslant i_4 \leqslant i_3 \leqslant n-i$.

In Sec. IV we have used a different expansion of $[f(x)]^n$. In this case we expand $[P(x)]^i$ as follows:

$$[P(x)]^i = \left[p_0 + \frac{p_1}{x} + \cdots + \frac{p_{s-1}}{x^{s-1}}\right]^i$$
$$= \sum \binom{i}{i_1} \cdots \binom{i_{s-2}}{i_{s-1}} \left(\frac{p_0}{p_1}\right)^{i_{s-1}}$$
$$\times \cdots \left(\frac{p_{s-2}}{p_{s-1}}\right)^{i_1} (p_{s-1})^i \frac{1}{x^{(s-1)i-p}}, \qquad \text{(C14)}$$

with the summation as in Eq. (C3). Similarly,

$$[Q(x)]^{n-i} = \left[q_0 + \frac{q_1}{x} + \cdots \frac{q_s}{x^s}\right]^{n-i}$$
$$= \sum \binom{n-i}{j_i} \cdots \binom{j_{s-1}}{j_s} \left(\frac{q_0}{q_1}\right)^{j_s} \cdots \left(\frac{q_{s-1}}{q_s}\right)^{j_1}$$
$$\times q_s^{\,n-1} \frac{1}{x^{s(n-i)-q}}, \qquad \text{(C15)}$$

with the summation as in Eq. (C4). Equations (C14) and (C15), together with the requirement $p_{s-1} = q_s$ (see Appendix B), give the alternative form of Eq. (C6),

$$(q_s)^n \sum_{i=0}^{n} \binom{n}{i} \binom{i_{s-2}}{i_{s-1}} \cdot \left(\frac{p_0}{p_1}\right)^{i_{s-1}}$$
$$\times \cdots \left(\frac{p_{s-2}}{p_{s-1}}\right)^{i_1}$$
$$\times \binom{n-i}{j_1} \cdots \binom{j_{s-1}}{j_s} \left(\frac{q_0}{q_1}\right)^{j_s}$$
$$\times \cdots \left(\frac{q_{s-1}}{q_s}\right)^{j_1} I_\epsilon(n-i,m). \qquad \text{(C16)}$$

Now with $m \equiv ns - p - q - 1 - t - i$, we will use the following compact notation:

$$\hat{\sum_1}(i) \equiv \sum \binom{i}{i_1} \cdots \binom{i_{s-2}}{i_{s-1}} \left(\frac{p_0}{p_1}\right)^{i_{s-1}}$$
$$\times \cdots \left(\frac{p_{s-2}}{p_{s-1}}\right)^{i_1},$$

and $\qquad \text{(C17)}$

$$\hat{\sum_2}(j_1) \equiv \sum \binom{j_1}{j_2} \cdots \binom{j_{s-1}}{j_s} \left(\frac{q_0}{q_1}\right)^{j_s}$$
$$\times \cdots \left(\frac{q_{s-2}}{q_{s-1}}\right)^{j_2},$$

where the hat "$\wedge$" reminds us that everything behind $\hat{\Sigma}_{1,2}$ depending on either the i_k's or j_k's is to be included in the sum. With this in mind, $\tilde{Z}(n,l)$, $R(n)$, and the divergent part $D(n)$ become

$$\tilde{Z}(n,l) = (-q_s)^n n! \sum_{i=0}^{n+1-l} \frac{(-1)^i}{i!} \hat{\sum_1}(i)$$
$$\times \sum_{j_1=0}^{n-i} \binom{n-j}{j_1} \left(\frac{q_{s-1}}{q_s}\right)^{j_1}$$
$$\times \hat{\sum_2}(j_1) \cdot \frac{1}{m!} \begin{bmatrix} n+1-l-i \\ m \end{bmatrix}, \qquad \text{(C18)}$$

$$R(n) = (q_s)^n \sum_{i=0}^{n} \binom{n}{i} \hat{\sum_1}(i)$$
$$\times \sum_{j_1=0}^{n-i} \binom{n-i}{j_1} \left(\frac{q_{s-1}}{q_s}\right)^{j_1}$$
$$\times \hat{\sum_2}(j_1) R(n-i,m), \qquad \text{(C19)}$$

and finally,

$$D(n) = (-\log \epsilon) D'(n,0) + \sum_{k=1}^{\infty} \frac{1}{\epsilon^k} \cdot \frac{1}{k} \cdot D'(n,k),$$

with

$$D'(n,k) = (-q_s)^n n! \sum_{i=0}^{n} \frac{(-1)^i}{i!}$$
$$\times \hat{\sum_1}(i) \sum_{j_1=0}^{n-i} \binom{n-i}{j_1} \left(\frac{q_{s-1}}{q_s}\right)^{j_1}$$
$$\times \hat{\sum_2}(j_1) \cdot \frac{1}{(m-k)!} \begin{bmatrix} n-i \\ m-k \end{bmatrix}. \qquad \text{(C20)}$$

Since Eq. (C1) is finite, we have

$$D'(m,k) = 0, \quad \text{for } k = 0,1,2,\cdots. \qquad \text{(C21)}$$

Notice by putting $l = 1$ in Eq. (C18) we find $\tilde{Z}(n,1) = D'(n,0) = 0$, that is, the coefficient of "$\zeta(1)$" is zero.

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Inverse scattering of the permittivity and permeability profiles of a plane stratified medium

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It is shown that the permittivity and permeability profiles of a lossless plane stratified medium can be uniquely determined from the reflection coefficient due to transverse electric plane waves at two angles of incidence and all the frequencies. The inverse scattering problem at oblique incidence is transformed to an equivalent inverse scattering problem at normal incidences. The latter is transformed to an inverse scattering problem for the one-dimensional Schrödinger equations, the solution of which is obtained by the Gel'fand–Levitan theory.

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INTRODUCTION

A transverse electric plane wave is obliquely incident upon a plane stratified half-space $z \geqslant 0$. Required is the permittivity profile and the permeability profile of the half-space $z \geqslant 0$ from the reflection coefficient at two angles of incidence and all the frequencies. This is a nonlinear inverse scattering problem.

For the time harmonic dependence e^{jwt}, Maxwell equations show that the electric field E satisfies the equation

$$[\nabla^2 + k^2\epsilon(z)\mu(z)]E(w,z,x) = \left[\frac{d}{dz}\log\mu(z)\right]\frac{\partial E(w,z,x)}{\partial z},$$
$$-\infty < z < \infty, \tag{1}$$

where $\nabla^2 \equiv \partial^2/\partial x^2 + \partial^2/\partial z^2$ is transverse Laplacian operator, $k = w/c$ is the free space wavenumber, where w is the radian frequency and c is the speed of light *in vacuo*, $\epsilon(z)$ is the dielectric constant profile (relative premittivity profile), and $\mu(z)$ is the relative permeability profile of the plane stratified medium $-\infty < z < \infty$.

If the half-space $z \leqslant 0$ is assumed to be a uniform air with $\epsilon(z) = 1$ and $\mu(z) = 1$, then, for an obliquely incident plane wave, the solution of Eq. (1) in the region $z < 0$ is given by

$$E(w,z,x) = e^{-jkx\sin\theta}\{e^{-jkz\cos\theta} + \rho(w,\theta)e^{+jkz\cos\theta}\} \tag{2}$$

where θ is the angle of incidence and $\rho(w,\theta)$ is the reflection coefficient.

The objective is to determine the dielectric constant profile $\epsilon(z)$, $z \geqslant 0$, and the relative permeability profile $\mu(z)$, $z \geqslant 0$, from the reflection coefficient at two angles of incident and all the frequencies $\rho(w,\theta_l)$, $l = 1,2$, $-\infty < w < \infty$.

In what follows, the inverse scattering problem at oblique incidence is transformed to an equivalent inverse scattering problem at normal incidence, for which the transformed medium is characterized only by a ficticious refractive index profile. The inverse scattering problem for the ficticious refractive index profile is next transformed via the Liouville transformation[1] to an inverse scattering problem in quantum mechanics where the potential of the one-dimensional Schrödinger equation is sought from the reflection coefficient; an inverse problem whose solution can be obtained by a procedure due to Kay[2] and Kay and Moses[3] which is based on the Gel'fand–Levitan theory.[4] Knowing the reflection coefficient at two angles of incidence and all the frequencies allows the reconstruction of two potentials. These potentials are transformed back to two ficticious refractive index profiles, and, subsequently, the permeability and permittivity profiles of half-space $z \geqslant 0$ are recovered.

TRANSFORMATION TO THE SCHRÖDINGER EQUATION

In this section Eq. (1) is transformed to the one-dimensional Schrödinger equation.

For $z \geqslant 0$

$$E(w,z,x) = \phi(w,z)e^{-jkx\sin\theta}, \tag{3}$$

and Eq. (1) shows that

$$\left\{\frac{\partial^2}{\partial z^2} + k^2[\epsilon(z)\mu(z) - \sin^2\theta]\right\}\phi(w,z) = \left[\frac{d}{dz}\log\mu(z)\right]\frac{\partial\phi(w,z)}{\partial z}. \tag{4}$$

Now, change the depth z to an "apparent depth" s, by the transformation

$$\frac{ds}{dz} = \mu(z). \tag{5}$$

Equation (4) is thus transformed to

$$\left[\frac{\partial^2}{\partial s^2} + k^2\alpha^2(s,\theta)\right]\phi(w,s) = 0, \quad s \geqslant 0, \tag{6}$$

where

$$\alpha^2(s,\theta) = \frac{1}{\mu^2(s)}[\epsilon(s)\mu(s) - \sin^2\theta]. \tag{7}$$

In the region $s < 0$, $\mu(z) = 1$, and Eqs. (2) and (3) show that

$$\phi(w,s) = e^{-jks\cos\theta} + \rho(w,\theta)e^{jks\cos\theta}, \quad s < 0. \tag{8}$$

A physical interpretation of Eqs. (6)–(8) is as follows: A plane stratified "refractive medium" occupies the region $-\infty < s < \infty$. The region $s < 0$ is homogeneous with a "refractive index" of $\cos\theta$ and the region $s \geqslant 0$ is inhomogeneous with a "refractive index" profile $\alpha(s,\theta)$. A plane wave is normally incident upon the inhomogeneous region from the ho-

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mogeneous region and $\rho(w,\theta)$ in the reflection coefficient.

The inverse scattering problem for the plane stratified "refractive medium" is as follows: Given the reflection coefficient $\rho(w,\theta)$, $-\infty < w < \infty$, and the "refractive index" of the homogeneous region $s<0$, what is the "refractive index" profile of the inhomogeneous region $s \geqslant 0$?

The solution of this inverse scattering problem is obtained by transforming Eq. (6) to the one-dimensional Schrödinger equation, whose potential can be recovered from the reflection coefficient.

The Liouville transformation[1]

$$\psi(w,\xi) = g(s)\phi(w,s), \quad \frac{ds}{d\xi} = g^{-2}(s), \quad g(s) = \alpha^{1/2}(s,\theta) \tag{9}$$

transforms Eq. (6) to the one-dimensional Schrödinger equation

$$\left(\frac{\partial^2}{\partial \xi^2} + \frac{w^2}{c^2}\right)\psi(w,\xi) = Q(\xi)\psi(w,\xi), \tag{10}$$

where the potential $Q(\xi)$ is given by

$$Q(\xi) = g^{-1}(\xi)\frac{\partial^2 g(\xi)}{\partial \xi^2}. \tag{11}$$

It will be noted that the mapping of Eq. (6) to the Schrödinger equation (10), by the Liouville transformation,[1] has been used also by Schelkunoff,[5] Moses and deRidder,[6] Ware and Aki,[7] and Sharp.[8] This mapping requires, however, that the "refractive index" profile $\alpha(s,\theta)$ is a continuous function of s.

Following Kay,[2] Kay and Moses,[3] and Gel'fand and Levitan,[4] the refractive index profile $\alpha(s,\theta)$, $s \geqslant 0$, is obtained from the reflection coefficient $\rho(w,\theta)$, $-\infty < w < \infty$, as follows:

1. $R(\xi) = \dfrac{1}{2\pi}\displaystyle\int_{-\infty}^{\infty} \rho(w,\theta)e^{iw\xi}dw,$
2. $K(\xi,\tau) = -R(\xi+\tau) - \displaystyle\int_{-\xi}^{\xi} K(\xi,\sigma)R(\sigma+\tau)d\sigma,$
   $|\tau| \leqslant \xi, \ \xi \geqslant 0,$
3. $g(\xi) = g(0)\left[1 + \displaystyle\int_{-\xi}^{\xi} K(\xi,\tau)d\tau\right],$
4. $s = \displaystyle\int_0^{\xi} g^{-2}(\xi')d\xi',$
5. $\alpha(s,\theta) = g^2(\xi(s)).$

It will be noted that $\xi = \xi(s)$ has a unique inverse $s = s(\xi)$ provided that $\alpha(s,\theta)$ as given by Eq. (7) is positive for all $0 \leqslant s < \infty$.

The algorithm 1–5 requires that the potential $Q(\xi)$ be piecewise continuous and in addition that $\int_0^\infty (1+|\xi|)|Q(\xi)|d\xi < \infty$, which imposes additional restrictions on the "refractive index" profile $\alpha(s,\theta)$

INVERSION OF THE PERMEABILITY AND PERMITTIVITY PROFILES

In this section the permeability profile $\mu(z)$ and permittivity profile $\epsilon(z)$ of the half space $z \geqslant 0$ are obtained from the data $\rho(w,\theta_l)$, $l = 1,2$ and $-\infty < w < \infty$.

The inversion procedure given in the previous section is applies to the reflection coefficient $\rho(w,\theta_1)$ and then to $\rho(w,\theta_2)$. This will result with the two "refractive index" profiles $\alpha(s,\theta_1)$ and $\alpha(s,\theta_2)$. Equation (7) now shows that

$$\mu^2(s) = \frac{\sin^2\theta_1 - \sin^2\theta_2}{\alpha^2(s,\theta_2) - \alpha^2(s,\theta_1)} \tag{12}$$

and

$$\epsilon(s) = \frac{\mu^2(s)\alpha^2(s,\theta_1) + \sin^2\theta_1}{\mu(s)}. \tag{13}$$

So, the permeability and permittivity profiles have been determined as a function of the "apparent depth" s.

Equation (5) now shows that

$$z = \int_0^s \frac{ds'}{\mu(s')}, \tag{14}$$

which gives the relationship between "apparent depth" s and the actual depth z. Note that because $\mu(z) > 0$, $z = z(s)$, is a monotonically increasing function whose inverse $s = s(z)$ is unique.

Equations (12) and (13) raise the following question[9]: If one prescribes the reflection coefficient $\rho(w,\theta)$ for $\theta = \theta_1$, $\theta = \theta_2$ and obtains $\mu^2(s)$ and $\epsilon(s)$, under what conditions would $\mu^2(s)$ and $\epsilon(s)$ be independent of the choices of θ_1 and θ_2? The conditions are that $\epsilon(z)$ and $\mu(z)$ should be twice differentiable and together with the angles of incidence satisfy

$$\epsilon(z)\ \mu(z) - \sin^2\theta_l > 0, \quad l = 1, 2, \quad -\infty < z < \infty \tag{15a}$$

and

$$\int_0^\infty [1 + |\xi|]|Q(\xi)|d\xi < \infty, \tag{15b}$$

where $Q(\xi)$ is related to $\mu(\xi)$, $\epsilon(\xi)$, and θ by Eqs. (11), (9), and (7). These will allow the unique reconstructions of the "refractive index" profiles $\alpha(s,\theta_1)$ and $\alpha(s_1,\theta_2)$. If, in addition, $\mu(z)$ and $\epsilon(z)$ are positive-valued functions, then their reconstruction by Eq. (12) and (13) will be θ-independent, and therefore they are uniquely recovered from the reflection coefficients $\rho(w,\theta_l)$, $l = 1,2$, $-\infty < w < \infty$.

DISCUSSION

It was shown in this paper that the permeability and premittivity profiles of a layered medium can be uniquely recovered from the reflection coefficient due to a transverse electric plane wave at two angles of incidence and all the frequencies. A direct (noniterative) inversion algorithm has been developed which constructs these profiles from the reflection coefficient data. The angles of incidence must satisfy condition 15(a), which by Snell's law means that the critical angle is not reached at any point within the medium. If the critical angle is reached at some critical depth $z = z_c$, then there will be no leakage of energy beyond the critical depth and the magnitude of the reflection coefficient $|\rho(w,\theta)| = 1$ for all frequencies. In this case the information about the medium $0 < z < z_c$ is contained in the phase of the reflection coefficient $\arg\{\rho(w,\theta)\}$. There are two possibilities, either the critical angle is reached by one angle of incidence at $z = z_c$ or it is reached by both angles of incidence at $z = z_{c_1}$

and $z = z_{c_2}$, respectively. In the former case the permeability and permittivity profiles can be reconstructed up to $z = z_c$ whereas in the later case they are reconstructed up to min $\{z_{c_1}, z_{c_2}\}$. It will be concluded that the critical angle is not reached for transverse electric polarization when $\epsilon(z)$, $\mu(z) \geqslant 1, \quad 0 < z < \infty$.

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Propagation of the fourth-order coherence function in an anisotropic random medium

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The propagation of the fourth-order coherence function through an anisotropic random medium is investigated for low frequency radiation using the parabolic approximation and perturbation techniques. Theoretical expressions are derived for the intensity fluctuations and correlations of an initial plane wave signal that has propagated a horizontal distance z into the medium. The expressions are valid for anisotropic media in which $kl_H \gg 1$ and $kl_V^2/l_H \ll 1$, where k is the radiation wavenumber, l_H and l_V are, respectively, characteristic correlation lengths parallel and perpendicular to the propagation direction z. The results are compared to those obtained for an isotropic random medium.

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1. INTRODUCTION

We study here propagation of acoustic energy in an anisotropic random medium using coherence theory. Previous formulations utilize a two point coherence function $\{\hat{\Gamma}(\mathbf{x}_1, \mathbf{x}_2, \nu)\} = \{\hat{p}(\mathbf{x}_1, \nu)\hat{p}^*(\mathbf{x}_2, \nu)\}$ which is the ensembel average over the product of the complex acoustic pressure field (with frequency ν) and of its conjugate measured at two points located in a plane which is taken to be normal to the principal propagation direction. Equations that govern $\{\hat{\Gamma}(\mathbf{x}_1, \mathbf{x}_2, \nu)\}$ under various propagation conditions were derived by Beran and McCoy[1,2] and Tappert, *et al.*[3,4]

A knowledge of $\{\hat{\Gamma}(\mathbf{x}_1, \mathbf{x}_2, \nu)\}$ allows us to determine both the intensity distribution $\{I(\mathbf{x})\} = \{\hat{\Gamma}(\mathbf{x}, \mathbf{x}, \nu)\}$ and the angular spectrum of radiation (which is directly related to the resolution limitation resulting from the presence of the scattering medium).

From a coherence point of view, however, intensity fluctuations and correlations can be obtained only from a four-point (i.e., fourth-order) coherence function $\{\hat{L}\}$:

$$\{\hat{L}^1(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \nu)\} = \{\hat{p}(\mathbf{x}_1, \nu)\hat{p}^*(\mathbf{x}_2, \nu)\hat{p}^*(\mathbf{x}_3, \nu)\hat{p}(\mathbf{x}_4, \nu)\}. \quad (1)$$

The braces denote an ensemble average. The function $\{\hat{L}^1(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \nu)\}$ $(\mathbf{x}_1 = \mathbf{x}_2, \mathbf{x}_3 = \mathbf{x}_4)$ is the coherence of intensity fluctuations and is of importance in space diversity systems. The quantity $\{I^2(\mathbf{x})\} = \{\hat{L}^1(\mathbf{x}, \mathbf{x}, \mathbf{x}, \mathbf{x}, \nu)\}$ gives the intensity fluctuations in the received signal. Information about $\{I^2(x)\}$ is of importance in studying the noise in communication systems. (See Refs. 5, 6, and 7 for a study of fluctuations from an amplitude-phase point of view.)

The purpose of this paper is to treat the low frequency propagation of the fourth order coherence function $\{\hat{L}^1\}$ in an anisotropic random medium by employing the parabolic approximation of the wave equation and perturbation techniques similar to those of Ho and Beran.[8] We restrict our discussion to homogeneous random media.

The next section describes the properties of the medium that are relevant to our problem and explains why previous results in optics that have been obtained for $\{\hat{L}^1\}$ cannot be used here for low frequency propagation. In Sec. 3, the parabolic approximation is utilized to obtain general, second order, perturbation expressions for $\{\hat{L}^1\}$. Section 4 uses the results of Sec. 3 along with several approximations to derive solutions of $\{\hat{L}^1\}$ for an acoustic plane wave whose propagation direction is horizontal. In Sec. 5 we discuss propagation of an arbitrary spectrum of plane waves.

2. THE ANISOTROPIC NATURE OF TEMPERATURE FLUCTUATIONS IN THE OCEAN

The vertical temperature profile[9] of the ocean results in sound channels that can support "guided" waves for very large propagation distances. However, temperature fluctuations in these channels scatter the sound waves and cause reduction in the propagated energy, loss of coherence and intensity fluctuations of the acoustic radiation. In this paper we study this scattering with relation to intensity fluctuations in the absence of a sound channel. The results of this investigation may then be used as a basis for further study of the real ocean problem.

This paper considers the temperature microstructure as the only source of scattering of acoustic signals in the ocean. The fluctuations in the index of refraction that are associated with the temperature microstructure are random and, in general, very weak. The temperature microstructure in the ocean is very anisotropic, with correlation lengths defined by measurements taken in a horizontal direction being orders of magnitude greater than corresponding lengths defined by measurements taken in the depth direction. Typically, horizontal corelation lengths are of the order of kilometers and vertical correlation lengths are of the order of tens of meters.[10] Since the ocean has good transmission for low fre-

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quency acoustic signals ($\nu \leqslant 100$ Hz), typical (i.e. for practical long range propagation) wavenumbers (m^{-1}) are less than unity. The scattering theory presented in this paper is applicable to a highly anisotropic fluctuation field with frequency such that

$$kl_H \gg 1, \tag{2a}$$

$$kl_V^2/l_H \ll 1. \tag{2b}$$

Here k is the wavenumber ($= 2\pi\nu/c$); l_H and l_V are correlation lengths for measurements in a horizontal direction and the vertical direction, respectively. Typical values of k, l_H, and l_V in the ocean were quoted above, and it can be seen that they approximately fulfil the two conditions (2) for low frequencies. For example if $\nu = 50$ Hz ($k = 0.21$ m^{-1}), $l_V = 100$ m and $l_H = 10^4$ m; then $kl_V^2/l_H = 0.21$.

Intensity fluctuations of waves propagating in isotropic media have been extensively investigated. Several monographs and review articles[5,6,11,12,13] describe the current state of art. However, the assumption that $kl_V^2/l_H \ll 1$ is not in accordance with some of the approximations necessary for the validity of the isotropic results. In particular, the single scattering solution for an isotropic medium shows that the characteristic angular spread of the scattered radiation is $O(1/kl_m)$ (i.e. on the order of $1/kl_m$), l_m is the smallest correlation length and it is assumed that $kl_m \gg 1$. However, for low frequency propagation in the ocean, where $kl_H \gg 1$ and $kl_V^2/l_H \ll 1$, the characteristic angular spreads (for a plane wave propagating horizontally) in the horizontal and vertical planes, are given, respectively, by

$$\theta_H = O(1/kl_H),$$

$$\theta_V = O\left[(1/\sqrt{kl_H})\right]. \tag{3}$$

Thus for low-frequency propagation intensity fluctuations in the ocean cannot be predicted on the basis of isotropic theories.

3. MATHEMATICAL FORMULATION

A. Problem statement

We wish to study the propagation of low frequency acoustic signals over moderate propagation paths in a homogeneous anisotropic random medium. For convenience, we assume that the statistics of the refractive index field are isotropic in the horizontal plane. The problem geometry is given in Fig. 1. The XYZ coordinate system is fixed with respect to the medium, Y is the depth coordinate, Z is a horizontal range coordinate and X is a transverse coordinate. The propagation direction of the incident acoustic radiation coincides with the z axis which forms an angle θ with the XYZ system.

We assume that $\{\hat{L}^1(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \nu)\}_{z_1=z_2=z_3=z_4=z}$ is given at $z=0$ and consider the propagation into the $z>0$ region, $\{\hat{L}^1\}$ will be evaluated only for points $\mathbf{x}_i$ ($i = 1$–4) which lie in a plane perpendicular to the z axis. Thus

$$\begin{aligned}\{\hat{L}^1(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \nu)\}|_{z_1=z_2=z_3=z_4=z} &= \{\hat{L}^1(\mathbf{x}_{T_1}, \mathbf{x}_{T_2}, \mathbf{x}_{T_3}, \mathbf{x}_{T_4}, z, \nu)\} \\ &= \{\hat{p}(\mathbf{x}_{T_1}, z, \nu)\hat{p}^*(\mathbf{x}_{T_2}, z, \nu)\hat{p}^*(\mathbf{x}_{T_3}, z, \nu)\hat{p}(\mathbf{x}_{T_4}, z, \nu)\},\end{aligned} \tag{4}$$

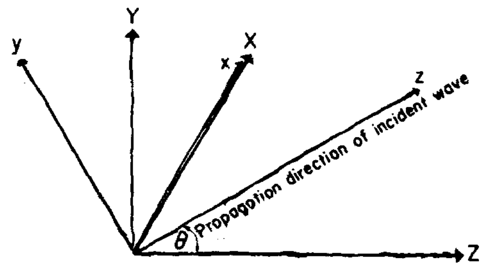

FIG. 1. Problem geometry. The $\{XYZ\}$ system is fixed with respect to the medium. The correlation length in the $\{XZ\}$ plane is l_H. The vertical correlation length is l_V.

$\mathbf{x}_{T_i} = (x_i, y_i)$ are transverse coordinates.

We now use perturbation theory and solve for $\hat{p}(\mathbf{x}_T, z, \nu)$ in terms of $\hat{p}(\mathbf{x}_T, 0, \nu)$ using an appropriate Green's function. The fourth order coherence function may then be formed from these functions using Eq. (4).

B. Perturbation solution

The governing wave equation is

$$\nabla^2\hat{p} + k^2[1+\mu]\hat{p} = 0, \tag{5}$$

where $\hat{p}(\mathbf{x}_T, z, \nu)$ is the complex acoustic pressure field, ν is the central frequency, and $k^2[1+\mu]$ ($= [2\pi\nu/c]^2$) is the square of the wave number. The wave number is written as the sum of an averaged value plus a random portion that averages to zero. We also assume that $\mu \ll 1$.

With no loss of generality we can write:

$$\hat{p}(\mathbf{x}_T, z, \nu) = b(\mathbf{x}_T, z, \nu)\exp(ikz). \tag{6}$$

Substituting Eq. (6) in Eq. (5), we get:

$$\nabla_T^2 b + \frac{\partial^2 b}{\partial z^2} + 2ik\frac{\partial b}{\partial z} + k^2\mu b = 0,$$

where $\nabla_T^2 = \partial^2/\partial x^2 + \partial^2/\partial y^2$ is the two-dimensional Laplacian operator defined for the z plane. If we restrict consideration to acoustic signals that have a narrow-angled spectrum centered about the z direction, we can neglect the second derivative term in z with respect to the first derivative term. The above approximation is referred to as the parabolic approximation and its validity is discussed in Refs. 14 and 15.

The resulting equation is

$$\nabla_T^2 b + 2ik\frac{\partial b}{\partial z} + k^2\mu b = 0. \tag{7}$$

Equation (7) can be converted to an integral equation in $\hat{p}(\mathbf{x}_T, z, \nu)$,

$$\begin{aligned}\hat{p}(\mathbf{x}_T, z, \nu) = \hat{p}_0(\mathbf{x}_T, z, \nu) &+ \frac{k^2}{4\pi}\exp(ikz) \\ &\times\int_0^z \frac{dz'}{z-z'}\iint_{-\infty}^{\infty} d\mathbf{x}'_T\mu(\mathbf{x}'_T, z'), \\ &\times\exp(-ikz')\hat{p}(\mathbf{x}'_T, z', \nu) \\ &\times\exp\left(\frac{ik[(x-x')^2+(y-y')^2]}{2(z-z')}\right).\end{aligned} \tag{8}$$

$\hat{p}_0(\mathbf{x}_T, z, \nu)$ is the solution when $\mu = 0$. We define an operator

H:

$$Hf(\mathbf{x}_T,z) = \frac{k^2}{4\pi}\exp(ikz)\int_0^z \frac{dz'}{z-z'} \times \iint_{-\infty}^{\infty} d\mathbf{x}'_T\, \mu(\mathbf{x}'_T, z')\exp(-ikz'),$$

$$f(\mathbf{x}'_T, z', \nu)\exp\left(\frac{ik\,[(x-x')^2+(y-y')^2]}{2(z-z')}\right).$$

In terms of H Eq. (8) becomes

$$\hat{p} = \hat{p}_0 + H\hat{p}. \tag{9}$$

Proceeding to second order perturbations using Eq. (9) we obtain

$$\hat{p} = \hat{p}_0 + H\hat{p}_0 + H^2\hat{p}_0 = \hat{p}_0 + \hat{p}_1 + \hat{p}_2. \tag{10}$$

$\hat{p}_1 \equiv H\hat{p}_0 = O(\mu)$ and $\hat{p}_2 \equiv H^2\hat{p}_0 = O(\mu^2)$. Substituting Eq. (10) into Eq. (4) gives

$$\begin{aligned}\{\hat{L}^1(\mathbf{x}_{T_1}, \mathbf{x}_{T_2}, \mathbf{x}_{T_3}, \mathbf{x}_{T_4}, z, \nu)\} &= \{[\hat{p}_0(\mathbf{x}_{T_1}, z, \nu) + \hat{p}_1(\mathbf{x}_{T_1}, z, \nu) + \hat{p}_2(\mathbf{x}_{T_1}, z, \nu)] \\ &\quad \times [\hat{p}_0^*(\mathbf{x}_{T_2}, z, \nu) + \hat{p}_1^*(\mathbf{x}_{T_2}, z, \nu) + \hat{p}_2^*(\mathbf{x}_{T_2}, z, \nu)] \\ &\quad [p_0^*(\mathbf{x}_{T_3}, z, \nu) + \hat{p}_1^*(\mathbf{x}_{T_3}, z, \nu) + \hat{p}_2^*(\mathbf{x}_{T_3}, z, \nu)] \\ &\quad [\hat{p}_0(\mathbf{x}_{T_4}, z, \nu) + \hat{p}_1(\mathbf{x}_{T_4}, z, \nu) + \hat{p}_2(\mathbf{x}_{T_4}, z, \nu)]\}.\end{aligned} \tag{11}$$

Equation (11) is expanded neglecting terms smaller than μ^2:

$$\begin{aligned}\{\hat{L}^1\}|_z &= \{\hat{L}_0^1\} + \{\hat{L}_{2000}\} + \{\hat{L}_{0200}\} + \{\hat{L}_{0020}\} + \{\hat{L}_{0002}\} \\ &\quad + \{\hat{L}_{1100}\} + \{\hat{L}_{1010}\} + \{\hat{L}_{0101}\} + \{\hat{L}_{0011}\} \\ &\quad + \{\hat{L}_{1001}\} + \{\hat{L}_{0110}\},\end{aligned} \tag{12}$$

where

$$\{\hat{L}^1\}|_z = \{\hat{L}^1(\mathbf{x}_{T_1}, \mathbf{x}_{T_2}, \mathbf{x}_{T_3}, \mathbf{x}_{T_4}, z, \nu)\},$$

$$\{\hat{L}_0^1\} = \{\hat{L}_{0000}\},$$

$$\{\hat{L}_{ijkl}\} = \{\hat{p}_i\hat{p}_j^*\hat{p}_k^*\hat{p}_l\}, \quad 0 \leqslant i,j,k,l \leqslant 2.$$

The $\hat{p}_i$ are defined in Eq. (10).

We shall give now specific expressions for $\{\hat{L}_{2000}\}$, $\{\hat{L}_{1100}\}$, and $\{\hat{L}_{1001}\}$ since all other terms (except $\{\hat{L}_0^1\}$) can then be evaluated by change of arguments.

$$\begin{aligned}\{\hat{L}_{2000}\} &= \frac{k^4}{(4\pi)^2}\exp(ikz)\int_0^z \frac{dz'}{z-z'}\int_0^{z'} \frac{dz''}{z'-z''}\iint_{-\infty}^{\infty} d\mathbf{x}'_T \iint_{-\infty}^{\infty} d\mathbf{x}''_T \sigma(\mathbf{x}', \mathbf{x}'')\exp\left(\frac{ik\,[(x_1-x')^2+(y_1-y')^2]}{2(z-z')}\right) \\ &\quad \times\exp\left(\frac{ik\,[(x'-x'')^2+(y'-y'')^2]}{2(z'-z'')}\right)\exp(-ikz'')\times\{\hat{L}_0^1(\mathbf{x}'', \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \nu)\},\end{aligned} \tag{13a}$$

$$\begin{aligned}\{\hat{L}_{1100}\} &= \frac{k^4}{(4\pi)^2}\int_0^z \frac{dz'}{z-z'}\int_0^z \frac{dz''}{z-z''}\iint_{-\infty}^{\infty} d\mathbf{x}'_T \iint_{-\infty}^{\infty} d\mathbf{x}''_T \sigma(\mathbf{x}', \mathbf{x}'') \\ &\quad \times\exp\left(\frac{ik\,[(x_1-x')^2+(y-y')^2]}{2(z-z')} - \frac{ik\,[(x_2-x'')^2+(y_2-y'')^2]}{2(z-z'')}\right) \\ &\quad \times\exp[-ik(z'-z'')]\{\hat{L}_0^1(\mathbf{x}', \mathbf{x}'', \mathbf{x}_3, \mathbf{x}_4, \nu)\},\end{aligned} \tag{13b}$$

$$\begin{aligned}\{\hat{L}_{1001}\} &= \frac{k^4}{(4\pi)^2}\exp(2ikz)\int_0^z \frac{dz'}{z-z'}\int_0^z \frac{dz''}{z-z''}\iint_{-\infty}^{\infty} d\mathbf{x}'_T \iint_{-\infty}^{\infty} d\mathbf{x}''_T \sigma(\mathbf{x}', \mathbf{x}'') \\ &\quad \times\exp\left(\frac{ik\,[(x_1-x')+(y_1-y')^2]}{2(z-z')} + \frac{ik\,[(x_4-x'')+(y_4-y'')^2]}{2(z-z'')}\right) \\ &\quad \times\exp[-ik(z'+z'')]\{\hat{L}_0^1(\mathbf{x}', \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}'', \nu)\},\end{aligned} \tag{13c}$$

where

$$\sigma(\mathbf{x}', \mathbf{x}'') = \sigma(\mathbf{x}'-\mathbf{x}'') = \{\mu(\mathbf{x}'_T, z')\mu(\mathbf{x}''_T, z'')\} \tag{14}$$

is the correlation function of the homogeneous temperature microstructure field. In deriving Eq. (13) we assumed that $\{\hat{L}_0^1\}$ is statistically independent of the refractive index field. In our problem this assumption is justified since $\{\hat{L}_0^1\}$ is governed by a wave equation and boundary conditions which do not contain μ.

In the following sections we evaluate Eq. (13) for various propagation conditions.

4. PLANE WAVE, HORIZONTAL PROPAGATION

When the unperturbed acoustic radiation is due to a plane wave propagating in the z direction, $\{\hat{L}_0^1\}$ is given by:

$$\{\hat{L}_0^1(\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, \mathbf{x}_4, \nu)\} = I^2\exp[ik(z_1-z_2-z_3+z_4)]. \tag{15}$$

I is the acoustical intensity.

In subsections 4A, 4B, and 4C we evaluate Eqs. (13a), (13b), and (13c), respectively. In subsection 4D we collect the results and study their nature.

A. $\{\hat{L}_{2000}\}$

We introduce new coordinates

$$\mathbf{s} = \mathbf{x}' - \mathbf{x}'', \qquad \mathbf{u} = \mathbf{x}'. \tag{16}$$

Using Eqs. (14)–(16), Eq. (13a) reduces to

$$\{\hat{L}_{2000}\} = \frac{k^4 I^2}{(4\pi)^2}\int_0^z \frac{du_z}{z-u_z}\int_0^{u_z}\frac{ds_z}{s_z}\iint_{-\infty}^{\infty} d\mathbf{u}_T$$

$$\times \iint_{-\infty}^{\infty} d\mathbf{s}_T \sigma(\mathbf{s}_T, s_z)$$

$$\times \exp\left(\frac{ik\,[(x_1-u_x)^2+(y_1-u_y)^2]}{2(z-u_z)} + \frac{ik\,[s_x{}^2+s_y{}^2]}{2s_z}\right). \quad (17)$$

Integration over $\mathbf{u}_T$ yields

$$\{\hat{L}_{2000}\} = \frac{ik^3 I^2}{8\pi}\int_0^z du_z \int_0^{u_z}\frac{ds_z}{s_z}\iint_{-\infty}^{\infty} d\mathbf{s}_T\, \sigma(\mathbf{s}_T, s_z)$$

$$\times \exp\left[+\frac{ik\,[s_x{}^2+s_y{}^2]}{2s_z}\right]. \quad (18)$$

For horizontal propagation, the term $(ks_x{}^2)/(2s_z)$ is of order kl_H. It was assumed, Eq. (2a), that $kl_H \gg 1$. Thus $\exp(iks_x{}^2/2s_z)$ oscillates very rapidly for $s_x \neq 0$ and the only contribution to the integral over s_x comes from the neighborhood of $s_x = 0$, where $\sigma(s_x, s_y, s_z) \approx \sigma(0, s_y, s_z)$. Moreover $ks_y{}^2/2s_z$ is of order of kl_V^2/l_H and according to Eq. (2b) is much smaller than unity, i.e., $\exp(iks_y{}^2/2s_z) \approx 1$.

Therefore

$$\{\hat{L}_{2000}\} = \frac{ik^3 I^2}{8\pi}\int_0^z du_z \int_0^{u_z}\frac{ds_z}{s_z}\int_{-\infty}^{\infty} ds_y\, \sigma(0, s_y, s_z)$$

$$\times \int_{-\infty}^{\infty} ds_x \exp\left(\frac{iks_x{}^2}{2s_z}\right), \quad (19)$$

and after integration over s_x

$$\{\hat{L}_{2000}\} = (-1+i)I^2\frac{k^{5/2}}{8(\pi)^{1/2}}\int_0^z du_z \int_0^{u_z}\frac{ds_z}{(s_z)^{1/2}}$$

$$\times \int_{-\infty}^{\infty} ds_y\, \sigma(0, s_y, s_z). \quad (20)$$

Integrating by parts over u_z gives us

$$\{\hat{L}_{2000}\} = (-1+i)I^2\frac{k^3}{8\sqrt{\pi}}\int_0^z \frac{ds_z(z-s_z)}{\sqrt{ks_z}}$$

$$\times \int_{-\infty}^{\infty} ds_y\, \sigma(0, s_y, s_z).$$

$\int_{-\infty}^{\infty} \sigma(0, s_y, s_z)\, ds_y$ is significant only for $|s_z| \lesssim l_H$. We shall assume that

$$z \gg l_H \quad (21)$$

and therefore

$$\{\hat{L}_{2000}\} = (-1+i)I^2\frac{k^3}{8\sqrt{\pi}}z\int_0^{\infty} \frac{ds_z}{\sqrt{ks_z}}$$

$$\times \int_{-\infty}^{\infty} ds_y\, \sigma(0, s_y, s_z); \quad (22)$$

In their paper on the propagation of the second order coherence function through anisotropic media,[1] Beran and McCoy have defined a scattering function $\bar{\sigma}_2(x_{12}, y_{12})$ which is given by

$$\bar{\sigma}_2(x_{12}, y_{12}) = \left(\frac{2}{\pi}\right)^{1/2}\frac{k^3}{4}\int_0^{\infty}\cos\left(\frac{ky_{12}^2}{2s_z} - \frac{\pi}{4}\right)\frac{\sigma_2(x_{12}, s_z)}{(ks_z)^{1/2}}ds_z, \quad (23a)$$

$$\sigma_2(x_{12}, s_z) = \int_{-\infty}^{\infty} ds_y\, \sigma(x_{12}, s_y, s_z), \quad (23b)$$

$x_{12} = x_1 - x_2, \quad y_{12} = y_1 - y_2.$

Rewriting Eq. (22) in terms of $\bar{\sigma}_2$, we have finally

$$\{\hat{L}_{2000}\} = \tfrac{1}{2}(-1+i)I^2\bar{\sigma}_2(0,0)z \quad (24)$$

and

$$\{\hat{L}_{2000}\} + \{\hat{L}_{0200}\} + \{\hat{L}_{0020}\} + \{\hat{L}_{0002}\} = -2I^2\bar{\sigma}_2(0,0)z. \quad (25)$$

B. $\{\hat{L}_{1100}\}$

$\sigma(\mathbf{x}' - \mathbf{x}'')$ can be represented as a transverse Fourier integral:

$$\sigma(\mathbf{x}' - \mathbf{x}'') = \iint_{-\infty}^{\infty} d\eta_x\, d\eta_y\, \tilde{\sigma}(n_x, n_y, z'-z'')$$

$$\times \exp[-i\eta_x(x''-x') - i\eta_y(y''-y')]. \quad (26)$$

Substituting Eq. (26) into Eq. (13b) using Eq. (15) yields

$$\{\hat{L}_{1100}\} = \frac{k^4 I^2}{(4\pi)^2}\int_0^z \frac{dz'}{z-z'}\int_0^z \frac{dz''}{z-z''}$$

$$\times \iint_{-\infty}^{\infty} d\eta_x\, d\eta_y\, \tilde{\sigma}(\boldsymbol{\eta}_T, z'-z'')$$

$$\times \iint_{-\infty}^{\infty} d\mathbf{x}'_T \iint_{-\infty}^{\infty} d\mathbf{x}'_T$$

$$\times \exp[-i\eta_x(x''-x') - i\eta_y(y''-y')]$$

$$\times \exp\left(\frac{ik\,[(x_1-x')^2+(y_1-y')^2]}{2(z-z')} - \frac{ik\,[(x_2-x')^2+(y_2-y')^2]}{2(z-z'')}\right), \quad (27)$$

where $\boldsymbol{\eta}_T = (\eta_x, \eta_y)$.

The integrations over x', y', x'', y'' may be performed by using the Fresnel integral. We use Eq. (16) and find

$$\{\hat{L}_{1100}\} = \frac{k^2 I^2}{4}\int_0^z du_z \int_{u_z-z}^{u_z} ds_z \iint_{-\infty}^{\infty} d\eta_x\, d\eta_y\, \tilde{\sigma}(\boldsymbol{\eta}_T, s_z)$$

$$\times \exp[i\eta_x(x_1-x_2) + i\eta_y(y_1-y_2)]$$

$$\cdot \exp\left[i\frac{(\eta_x^2+\eta_y^2)}{2k}s_z\right]. \quad (28)$$

For horizontal propagation, the term $(\eta_x^2 s_z)/(2k)$ is of order $l_H/(2kl_H^2) = 1/(2kl_H) \ll 1$, and $\exp(i\eta_x^2 s_z/2k) \approx 1$. On the other hand, $\eta_y^2 s_z/2k \approx l_H/2kl_V^2 \gg 1$, and therefore, $\exp(i\eta_y^2 s_z/2k)$ oscillates so rapidly for $n_y \neq 0$, that we may substitute $\tilde{\sigma}(\eta_x, \eta_y = 0, s_z)$ for $\tilde{\sigma}(\eta_x, \eta_y, s_z)$.

Thus

$$\{\hat{L}_{1100}\} = \tfrac{1}{4}(k^2 I^2)\int_0^z du_z \int_{u_z-z}^{u_z} ds_z \int_{-\infty}^{\infty} d\eta_x \tilde{\sigma}(\eta_x, 0, s_z)$$

$$\times \exp[i\eta_x(x_1-x_2)]$$

$$\times \int_{-\infty}^{\infty} d\eta_y \exp(i\eta_y^2 s_z/2k)\exp[i\eta_y(y_1-y_2)]. \quad (29)$$

Next we note that

$$\int_{-\infty}^{\infty} d\eta_y \exp\left(\frac{i\eta_y^2 s_z}{2k}\right)\exp[i\eta_y(y_1-y_2)]$$

$$= \left(\frac{2\pi}{k|s_z|}\right)^{\frac{1}{2}}\exp\left[\pm i\left(\frac{\pi}{4} - \frac{k(y_1-y_2)^2}{2|s_z|}\right)\right] \quad (30a)$$

(the upper sign corresponds to $s_z > 0$ and the lower sign to $s_z < 0$) and

$$\int_{-\infty}^{\infty} d\eta_x\, \tilde{\sigma}(\eta_x, 0, s_z)\exp[i\eta_x(x_1 - x_2)] = (1/2\pi)\sigma_2(x_{12}, s_z)$$

$$(x_{12} = x_1 - x_2). \tag{30b}$$

Substituting Eqs. (30a) and (30b) into Eq. (29), we have

$$\{\hat{L}_{1100}\} = I^2\left(\frac{2}{\pi}\right)^{\frac{1}{2}}\frac{k^3}{8}\int_0^z du_z \int_{u_z - z}^{u_z} ds_z \times\exp\left[\pm i\left(\frac{\pi}{4} - \frac{ky_{12}^2}{2|s_z|}\right)\right]\frac{\sigma_2(x_{12}, s_z)}{(k\,|s_z|)^{1/2}}$$

or

$$\{\hat{L}_{1100}\} = I^2\left(\frac{2}{\pi}\right)^{\frac{1}{2}}\frac{k^3}{8}\int_0^z (z - s_z)\frac{\sigma_2(x_{12}, s_z)}{(k\,|s_z|)^{1/2}}$$

$$\times\left\{\exp\left[-i\left(\frac{\pi}{4} - \frac{ky_{12}^2}{2|s_z|}\right)\right] + \exp\left[i\left(\frac{\pi}{4} - \frac{ky_{12}^2}{2|s_z|}\right)\right]\right\}ds_z. \tag{31}$$

The last expression was obtained after integration by parts followed by several manipulations. [By virtue of the horizontal isotropy we assumed $\sigma_2(x_{12}, s_z) = \sigma_2(x_{12}, -s_z)$]. Using the arguments that precede Eq. (24), we finally obtain

$$\{\hat{L}_{1100}\} = I^2\left(\frac{2}{\pi}\right)^{\frac{1}{2}}\frac{k^3}{4}z\int_0^\infty ds_z \cos\left(\frac{ky_{12}^2}{2s_z} - \frac{\pi}{4}\right)\frac{\sigma_2(x_{12},s_z)}{(ks_z)^{\frac{1}{2}}}$$

or

$$\{\hat{L}_{1100}\} = I^2\bar{\sigma}_2(x_{12}, y_{12})z \tag{32a}$$

and

$$\{\hat{L}_{1100}\} + \{\hat{L}_{1010}\} + \{\hat{L}_{0101}\} + \{\hat{L}_{0011}\} = I^2[\bar{\sigma}_2(x_{12}, y_{12}) + \bar{\sigma}_2(x_{13}, y_{13}) + \bar{\sigma}_2(x_{24}, y_{24}) + \bar{\sigma}_2(x_{34}, y_{34})]z \tag{32b}$$

$$(x_{ij} = x_i - x_j, y_{ij} = y_i - y_j).$$

C. $\{\hat{L}_{1001}\}$

Substituting Eqs. (15) and (26) into (13c) and integrating over x', y', x'', y'', we find

$$\{\hat{L}_{1001}\} = -\tfrac{1}{4}k^2I^2\iint_{-\infty}^{\infty} d\eta_x\, d\eta_y \int_0^z dz' \int_0^z dz''\exp(i\eta_x x_{14} + i\eta_y y_{14}) \times\tilde{\sigma}(\boldsymbol{\eta}_T, z' - z'')\exp\left[i\frac{(\eta_x^2 + \eta_y^2)}{2k}(z' - z) + i\frac{(\eta_x^2 + \eta_y^2)}{2k}(z'' - z)\right], x_{14} = x_1 - x_4, \quad y_{14} = y_1 - y_4.$$

In terms of the variables in Eq. (16) we have

$$\{\hat{L}_{1001}\} = -\tfrac{1}{4}k^2I^2\iint_{-\infty}^{\infty} d\eta_x\, d\eta_y\, \exp(i\eta_x x_{14} + i\eta_y y_{14})\times\exp\left[-i\frac{(\eta_x^2 + \eta_y^2)}{k}z\right]\int_0^z du_z\, \exp\left[i\frac{(\eta_x^2 + \eta_y^2)}{k}u_z\right] \times\int_{u_z - z}^{u_z} ds_z\, \tilde{\sigma}(\boldsymbol{\eta}_T, s_z)\exp\left[-i\frac{(\eta_x^2 + \eta_y^2)}{2k}s_z\right]. \tag{33}$$

The following discussion is valid only for horizontal propagation. Using integration by parts and incorporating horizontal isotropy, it can be shown that

$$\exp\left[-i\frac{(\eta_x^2 + \eta_y^2)}{k}z\right]\int_0^z du_z\, \exp\left[i\frac{(\eta_x^2 + \eta_y^2)}{k}u_z\right]\int_{u_z - z}^{u_z} \tilde{\sigma}(\boldsymbol{\eta}_T, s_z)\exp\left[-i\frac{(\eta_x^2 + \eta_y^2)}{2k}s_z\right] ds_z$$

$$= 2\int_0^z ds_z\, \tilde{\sigma}(\boldsymbol{\eta}_T, s_z)\exp\left[-\frac{i(\eta_x^2 + \eta_y^2)}{2k}s_z\right]\left(\frac{1 - \exp\{-i[(\eta_x^2 + \eta_y^2)/k\,](z - s_z)\}}{i(\eta_x^2 + \eta_y^2)/k}\right). \tag{34}$$

Substituting Eq. (34) into Eq. (33) we obtain

$$\{\hat{L}_{1001}\} = -\tfrac{1}{2}k^2I^2\int_0^z ds_z\, (z - s_z)\int_{-\infty}^{\infty} d\eta_x\, \exp(i\eta_x x_{14})\int_{-\infty}^{\infty} d\eta_y\, \tilde{\sigma}(\eta_x, \eta_y, s_z)\exp(i\eta_y y_{14})\exp\left[-i\frac{(\eta_x^2 + \eta_y^2)}{2k}s_z\right] \times\left(\frac{1 - \exp\{-i[(\eta_x^2 + \eta_y^2)/k\,](z - s_z)\}}{i[(\eta_x^2 + \eta_y^2)/k\,](z - s_z)}\right). \tag{35}$$

Define ζ by

$$\eta_y = [k/(z - s_z)]^{1/2}\cdot\zeta.$$

The integral over η_y becomes

$$\left(\frac{k}{z - s_z}\right)^{1/2}\int_{-\infty}^{\infty} d\zeta\, \tilde{\sigma}\left(\eta_x, \left(\frac{k}{z - s_z}\right)^{1/2}\zeta, s_z\right)\exp\left[i\left(\frac{k}{z - s_z}\right)^{1/2}y_{14}\zeta\right]\exp\left(-i\frac{\eta_x^2 s_z}{2k}\right)\exp\left(-i\frac{s_z}{z - s_z}\zeta\right) \times\left(\frac{1 - \exp[-i\,\eta_x^2(z - s_z)/k - i\zeta^2]}{i\,\eta_x^2(z - s_z)/k + i\zeta^2}\right). \tag{36}$$

In order to simplify the evaluation of Eq. (36), we use Eqs. (2) and (21) and two further assumptions:

$$z/kl_H^2 \ll 1, \tag{37}$$

$$(ky_{14}^2/z)^{1/2} s_z/2z \ll 1. \tag{38}$$

[Equation (37) is not very restrictive and Eq. (38) may be shown to be consistent with the solution obtained.] We now note

$$(k/z - s_z)^{1/2} y_{14} \approx \left(\frac{k}{z}\right)^{1/2} y_{14}, \quad s_z/z \ll 1, \quad \frac{\eta_x^2 s_z}{2k} \ll 1, \quad \frac{\eta_x^2 (z - s_z)}{k} \ll 1.$$

Further, $\tilde{\sigma}(\eta_x, \eta_y, s_z)$ will appreciably differ from $\tilde{\sigma}(\eta_x, 0, s_z)$ only if $[k/(z - s_z)]^{1/2} \approx 1/l_V$. This means that

$$\zeta \approx (z/kl_V^2)^{1/2} \gg (l_H/kl_V^2)^{1/2} \gg 1.$$

Since the last term in Eq. (36) oscillates and decays with ζ^2, this term becomes dominant and the integral over η_y [Eq. (35)] reduces to

$$\left(\frac{k}{z - s_z}\right)^{1/2} \cdot \tilde{\sigma}(\eta_x, 0, s_z) \cdot \int_{-\infty}^{\infty} \exp\left[i\left(\frac{k}{z}\right)^{1/2} y_{14}\zeta\right] \times \frac{1 - \exp(-i\zeta^2)}{i\zeta^2} d\zeta$$

$$= \sqrt{2\pi}\left(\frac{k}{z - s_z}\right)^{1/2} \tilde{\sigma}(\eta_x, 0, s_z)\, F\left(\left(\frac{k}{z}\right)^{1/2} y_{14}\zeta\right), \tag{39}$$

$$F\left(\left(\frac{k}{z}\right)^{1/2} y_{14}\right) = \int_{-\infty}^{\infty} \exp\left[i\left(\frac{k}{z}\right)^{1/2} y_{14}\zeta\right] \times \frac{1 - \exp(-i\zeta^2)}{i\zeta^2} d\zeta. \tag{39a}$$

In particular,

$$F(0) = 1 - i.$$

The dependence of F on its argument is depicted in Fig. 2.

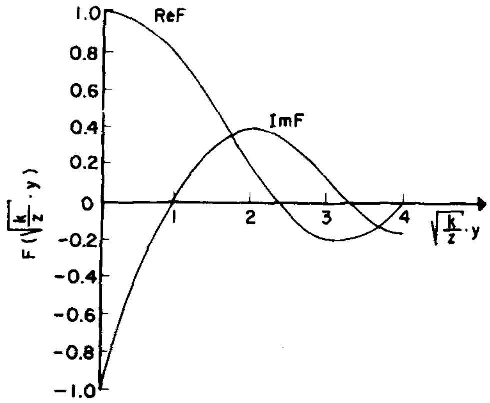

FIG. 2. The dependence of $F((k/z)^{1/2}y)$, Eq. (39a), on y. Note: F is an even function of y.

Substituting Eq. (39) into Eq. (35), using the expression

$$\int_{-\infty}^{\infty} d\eta_x \exp(i\eta_x x_{14})\tilde{\sigma}(\eta_x, 0, s_z) = (1/2\pi)\sigma_2(x_{14}, s_z),$$

we obtain

$$\{\hat{L}_{1001}\} = -(1/2\pi)(\pi/2)^{1/2} F((k/z)^{1/2} y_{14}) k^{5/2} I^2 \times \int_0^z ds_z\, (z - s_z)^{1/2} \sigma_2(x_{14}, s_z).$$

Since $z \gg l_H$, we have finally

$$\{\hat{L}_{1001}\} = -\hat{\sigma}_2(x_{14}, y_{14}) I^2 \sqrt{z}, \tag{40}$$

where

$$\hat{\sigma}_2(x_{14}, y_{14}) = \frac{k^{5/2} F((k/z)^{1/2} y_{14})}{\sqrt{8\pi}} \int_{-\infty}^{\infty} ds_z\, \sigma_2(x_{14}, s_z), \tag{41}$$

$$\{\hat{L}_{1001}\} + \{\hat{L}_{0110}\} = -I^2[\hat{\sigma}_2(x_{14}, y_{14}) + \hat{\sigma}_2^*(x_{23}, y_{23})]\sqrt{z}. \tag{41a}$$

The star denotes complex conjugation.

D. Study of theoretical results, Secs. 4A-4C

Adding Eqs. (25), (32), and (41), we obtain the final approximate expression for the propagation of $\{\hat{L}^1\}$ in the case of a plane wave which propagates in a horizontal direction

$$\{\hat{L}^1(\mathbf{x}_{T_1}, \mathbf{x}_{T_2}, \mathbf{x}_{T_3}, \mathbf{x}_{T_4}, z, \nu)\} = I^2\{1 + [\bar{\sigma}_2(x_{12}, y_{12}) + \bar{\sigma}_2(x_{13}, y_{13}) + \bar{\sigma}_2(x_{24}, y_{24}) + \bar{\sigma}_2(x_{34}, y_{34}) - 2\bar{\sigma}_2(0, 0)]z - [\hat{\sigma}_2(x_{14}, y_{14}) + \hat{\sigma}_2^*(x_{23}, y_{23})]\sqrt{z}\}. \tag{42}$$

The $\{\hat{L}_{1001}\}$ terms are of order $k^{5/2}\sigma(0, 0, 0)\, l_V\, l_H \sqrt{z}$ while the terms $\{\hat{L}_{2000}\}$ and $\{\hat{L}_{1100}\}$ are of order $k^{5/2}\sigma(0, 0, 0)\, l_V \sqrt{l_H}\, z$. Thus the $\{\hat{L}_{1001}\}$ terms are smaller by a factor of $(l_H/z)^{1/2}$ which was assumed to be small. It appears, therefore, that the last term in Eq. (42) [and also in Eq. (43)] can be neglected for $z \gg l_H$. We have decided, however, to keep the $\sqrt{z}$ terms in Eq. (42) since it may be shown that Eq. (42) gives good results even for $z/l_H \approx 2$, where omission of the $\sqrt{z}$ term would result in a gross error.

The coherence function of the intensity fluctuations (normalized by I^2) is defined by

$$C(x, y) = [\{I(x_1, y_1)I(x_1 + x, y_1 + y)\} - I^2]/I^2$$

$$\{I(x_1, y_1)I(x_1 + x, y_1 + y)\} = \hat{L}^1(\mathbf{x}_{T_1}, \mathbf{x}_{T_1}, \mathbf{x}_{T_3}, \mathbf{x}_{T_3}, z, \nu)\},$$

where

$$\mathbf{x}_{T_3} - \mathbf{x}_{T_1} = (x, y).$$

In this case, Eq. (42) yields

$$C(x, y) = 2[\bar{\sigma}_2(x, y)z - \mathrm{Re}(\hat{\sigma}_2(x, y))\sqrt{z}], \tag{43}$$

where $\mathrm{Re}[\hat{\sigma}_2]$ is the real part of $\hat{\sigma}_2$. The normalized intensity of fluctuations can be also obtained:

$$\sigma_I^2 = C(0, 0) = (\{I^2\} - I^2)/I^2 = 2[\bar{\sigma}_2(0, 0)z - \mathrm{Re}(\hat{\sigma}_2(0, 0))\sqrt{z}]. \tag{44}$$

Thus, for low frequency propagation we expect the intensity fluctuations to grow linearly with z (for large z/l_H). In the atmosphere, and in other isotropic media, intensity fluctuations of either sound or light waves grow with z^3.[6]

5. PROPAGATION IN AN ARBITRARY DIRECTION—ANGULAR SPECTRUM OF PLANE WAVES CENTERED ABOUT THE HORIZONTAL DIRECTION

Equations (13a)–(13c) may be used to study the propagation of a single plane wave in any arbitrary direction. We cannot obtain simple formulas like those in Eqs. (42) and (44) but σ_I^2 and $C(x, y)$ may be calculated numerically.

Similarly Eqs. (13a)–(13c) may be used to study the propagation of an angular spectrum of plane waves. Here, however, the angular spread must be small enough to justify use of the parabolic approximation which led to Eq. (7). This type of calculation is very important if we wish to carry the perturbation calculation to the next order where we calculate the rescattering of scattered waves. In this case the characteristic vertical angular spread of the scattered radiation is $\theta_V = O(1/(kl_H)^{1/2})$.

When this type of calculations was performed in the isotropic case,[16] where $\theta_V = O(1/kl)$ it was possible to show that $\Delta \{\hat{L}^{-1}\}$, over any interval where perturbation theory was applicable, was proportional to Δz. From this it was an easy matter to derive a partial differential equation which $\{\hat{L}^{1}\}$ satisfied over the whole region of propagation, whether it be the single scatter region or the multiple scatter region.

Here we have been unable to obtain such a relation because the approximations which are possible when $\theta_V = O(1/kl)$ are not possible when $\theta_V = O(1/(kl_H))^{1/2}$. Thus we have been unable to derive a partial differential equation governing $\{L^{1}\}$ which is dependent only on the second order correlation function.

We see again here that an anisotropic random medium for which $kl_V^2/l_H \ll 1$ behaves fundamentally differently from an isotropic random medium. The basic physics of the problem is changed by the strong anisotropy.

6. CONCLUSION

The purpose of this paper has been to study intensity fluctuations in low frequency propagation of acoustic radiation in an anisotropic random medium. Our treatment is confined to the perturbation region and we may expect it to be valid as long as the normalized intensity of fluctuations, σ_I^2 [Eq. (44)], is much smaller than unity. Moreover, in the real ocean [10], the thermal fluctuations are quite weak and σ_I^2 may remain smaller than 1 even for a propagation length of several tens of kilometers (for low enough frequencies).

We found that for propagation in the horizontal direction

$$\sigma_I^2 = 2\bar{\sigma}_2(0,0)z, \tag{45}$$

when $z/l_H \gg 1$, $kl_H \gg 1$ and $kl_V^2/l_H \ll 1$. Here l_H and l_V are characteristic correlation lengths in the horizontal and vertical directions, respectively, k is the radiation wavenumber, and z is the range. The function $\bar{\sigma}_2$ is defined by Eqs. (23) and depends upon the correlation of the speed of sound fluctuations.

The interesting fact about Eq. (45) is that σ_I^2 is proportional to z and not z^3 as it is in isotropic optical propagation studies. As a consequence, σ_I^2 is usually much greater than it would be if the speed of sound fluctuations were isotropic or if $kl_V^2/l_H \gg 1$ in addition to $kl_H \gg 1$.

We also found that because $\theta_V = O(1/(kl_H)^{1/2})$ and not $O(1/kl)$ as in the isotropic case, we could not obtain expressions for $\Delta \{\hat{L}^{1}\}$ that were linear in Δz when an angular spectrum of plane waves was present. The consequence of this is that we could not find a partial differential equation governing $\{\hat{L}^{1}\}$ which is dependent only on the second order correlation function.

We conclude on the basis of our results that there are fundamental differences in the behavior of a strongly anisotropic random medium ($kl_V^2/l_H \ll 1$) as compared to an isotropic random medium.

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ERRATA

Erratum: Partial inner product spaces III. Compatibility relations revisited [J. Math. Phys. 21, 268 (1980)]

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(1) Page 270, line 9 of 3.2 *Theorem* should read:

$\mathscr{F}(V,\#)$ is the complete...

(2) Page 272, line 6, left column, should read:

$$p < q \Rightarrow V_p \underset{\neq}{\subset} V_q.$$

(3) Page 275, line 5 of 5.1 *Example* should read:

$$f \#_2 g \quad \text{iff} \quad \sum_{n=0}^{\infty} n!|a_n b_n| < \infty.$$

(4) Page 276, line 17, right column, should read:

...i.e. $(V^{\#})^{\perp} = \{0\}$,...

(5) Page 277, line 18, right column: the formula should read:

$$T^{\beta} = \bigvee_{X``>T} X.$$

Erratum: A multigroup criticality condition for a space-independent multiplying assembly via the Chapman–Kolmogorov equation [J. Math. Phys. 21, 1897 (1980)]

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1. In (1) replace $\eta_2^{j_1}$ by $\eta_2^{j_2}$.
2. In (1) replace $\binom{j_2 - j_1}{j_2}$ by $\binom{j - j_1}{j_2}$.
3. In the unnumbered equation on line 15, p. 1900, left column, replace $x_{g'}$ by $x_{0g'}$.
4. In (39) replace $x_{g'}$ by $x_{0g'}$.