A folk theorem revisited: Degenerate representations

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It is known that when bases for generic irreducible representations of a semisimple group are reduced according to a semisimple subgroup the number of functionally independent missing label operators is just twice the number of missing labels. It is shown that the relation continues to hold when degenerate irreducible representations are considered.

I. INTRODUCTION

When a Lie group is applied to a physical problem, one often needs basis states of irreducible representations (IR's) of the group reduced according to IR's of a subgroup. Often the subgroup does not provide enough labels to specify the basis states completely.

One solution to this difficulty is to use the common eigenstates of a complete set of commuting operators as bases. Besides the Casimir invariants of group and subgroup, an appropriate number of "missing label" operators must be found; they should be subgroup invariants that are functions of the group generators.

Peccia and Sharp[1] showed that for generic IR's the number of missing label operators is exactly twice the number of missing labels; we follow Gilmore and Draayer[2] in referring to this result as the missing label folk theorem. Later Giroux, Couture, and Sharp[3] considered a number of specific examples dealing with degenerate representations (i.e., representations for which one or more Dynkin labels vanish). In each case the number of missing label operators was twice the number of missing labels. They conjectured that the folk theorem holds for degenerate, as well as for generic, IR's, but could not provide a proof. Such a proof, valid for semisimple groups, is the content of the present paper; it is a straightforward generalization of the proof given in Ref. 1 for generic IR's.

Gilmore and Draayer,[2] in a recent publication, have expressed a contrary opinion: "...a directly applicable criterion such as the missing label folk theorem would be useful ...(but) it fails for several applications considered above...we cannot recommend it as a test for completeness of an integrity basis." Gilmore and Draayer do not say for which of their applications the folk theorem fails; we have examined all the applications in their paper and found that the conjecture is valid for each case.

II. COUNTING MISSING LABELS AND MISSING LABEL OPERATORS

We consider a semisimple group G and a subgroup H. For those degenerate IR's of G for which specified Dynkin labels vanish the number of internal labels is known to be[4]

$$\tfrac{1}{2}(r_G - l_G - r_{G'} + l_{G'}), \tag{1}$$

where r and l denote order and rank, respectively. Here G' is the subgroup of G whose Dynkin diagram is obtained from that of G by retaining the nodes (and lines connecting them), corresponding to the zero Dynkin labels; it is the subgroup whose negative root generators annihilate highest weight states of the degenerate representations under consideration. To count missing labels we subtract the number of labels, Dynkin and internal, provided by H; that number is

$$\tfrac{1}{2}(r_H + l_H - r_{H'} - l_{H'}) - l'. \tag{2}$$

It may happen that only degenerate representations of H appear in the degenerate representations of G under consideration; then H' is the subgroup of H corresponding to *its* zero Dynkin labels; $l_H - l_{H'}$ is the number of nonzero Dynkin labels of H; l' is the number of G Casimirs which depend only on H generators. Thus the number of missing labels is

$$n = \tfrac{1}{2}(r_G - l_G - r_{G'} + l_{G'} - r_H - l_H + r_{H'} + l_{H'}) + l'. \tag{3}$$

Before counting missing label operators we must establish the number of functionally independent generators, or equivalently, group parameters in the case of degenerate IR's. This can be done by reversing an old argument due to Racah[5]; he reasoned that in the matrix elements $(q|U|s)$ the basis states $|s)$ and $|q)$ carry the same information as the group transformation U, and therefore depend on r parameters. Since $|s)$ and $|q)$ have the same values for the l Dynkin labels, but different values of the internal labels, say x in number, it follows that $r = l + 2x$. In our degenerate case the number of nonzero Dynkin labels is $l_G - l_{G'}$ and the number of independent internal labels is $\frac{1}{2}(r_G - l_G - r_{G'} + l_{G'})$. Thus the number of independent generators is

$$l_G - l_{G'} + 2\cdot\tfrac{1}{2}(r_G - l_G - r_{G'} + l_{G'}) = r_G - r_{G'}. \tag{4}$$

Similarly the number of independent H-generators is $r_H - r_{H'}$.

To determine the number of subgroup invariants, we envisage determining them by means of a device used by many authors,[6] i.e., solving a set of partial differential equations. The equations are those corresponding to the first $r_H - r_{H'}$ rows (i.e., to the independent subgroup generators) of the degenerate commutator table. The method of derivation shows that the number of subgroup scalars is $r_G - r_{G'} - R$, where R is the rank of the first $r_H - r_{H'}$ rows of the commutator table. Subtracting the number $l_G - l_{G'} + l_H - l_{H'} - l'$ of independent group/subgroup Casimir invariants we find the number of available missing label operators to be

$$m = r_G - r_{G'} - R - l_G + l_{G'} - l_H + l_{H'} + l'. \tag{5}$$

We want to show that $m = 2n$, i.e., that

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$$l' = r_H - r_{H'} - R. \tag{6}$$

But (6) follows from the definition of l': group scalars which depend only on subgroup generators are found by solving the $r_G - r_{G'}$ differential equations corresponding to the first $r_H - r_{H'}$ columns of the commutator table; because of antisymmetry the rank of the first $r_H - r_{H'}$ columns is the same as that of the first $r_H - r_{H'}$ rows.

III. EXAMPLES

We consider two examples, $SU(6) \supset SO(3)$ for the degenerate representations $(\lambda_1 0000)$ and $(\lambda_1 \lambda_2 000)$. These cases are considered in greater detail by Gilmore and Draayer. Here we simply count missing labels and missing label operators to check the validity of the folk theorem.

For $(\lambda_1 0000)$ IR's there are[4] $15 - 10 = 5$ internal labels needed; since SU(2) provides two there are three missing labels. For $(\lambda_1 \lambda_2 000)$ IR's there are[4] $15 - 6 = 9$ internal labels needed and hence seven missing labels.

Acting on degenerate IR's of a group G, the number of occurrences of an IR (λ) in the enveloping algebra is,[3] modulo multiplying by Casimirs, equal to the multiplicity in (λ) of the scalar IR of the subgroup $G' \times U(1) \times \cdots \times U(1)$, where G' is, as before, the subgroup corresponding to the vanishing Dynkin labels and the $l_G - l_{G'}$ subgroups U(1) span the directions of weight space orthogonal to G'.

For $(\lambda_1 0000)$ IR's the multiplicity of scalar $SU(5) \times U(1)$ IR's in SU(6) IR's is known from $SU(6) \supset SU(5) \times U(1)$ branching rules to be given by the generating function

$$(1 - \Lambda_1 \Lambda_5)^{-1}. \tag{7}$$

This means that the multiplicity of $SU(5) \times U(1)$ scalars in the IR (λ) and therefore the multiplicity of the IR (λ) in the degenerate enveloping algebra is the coefficient of $\Pi_{i=1}^{5} \Lambda_i^{\lambda_i}$ in the expansion of (7), i.e., unity for $(\lambda 000 \lambda)$, zero otherwise. Similarly, for $(\lambda_1, \lambda_2, 000)$ IR's the multiplicity of scalar $SU(4) \times U(1) \times U(1)$ IR's in the SU(6) IR (λ) is found from known branching rules[7] for $SU(6) \supset SU(4) \times SU(2) \times U(1)$. The result, which also gives the number of (λ) IR's in the corresponding degenerate enveloping algebra, is described by the generating function

$$[(1 - \Lambda_1 \Lambda_5)^2 (1 - \Lambda_2 \Lambda_4)]^{-1} \times [(1 - \Lambda_1^2 \Lambda_4)^{-1} + \Lambda_2 \Lambda_5^2 (1 - \Lambda_2 \Lambda_5^2)^{-1}]. \tag{8}$$

To count SO(3) scalars in the enveloping algebra for these two degenerate cases, it is convenient to count instead SU(3) IR's in the enveloping algebra, since each even–even SU(3) IR contains just one SO(3) scalar. To get a generating function for SU(3) IR's in the enveloping algebra, it is necessary to "substitute"[7] the $SU(6) \supset SU(3)$ branching rules generating function into the generating function (7) or (8). Since we care only about the number of SO(3) scalars, we do not need the relevant generating functions, but only the number of their denominator factors.

For the $(\lambda_1 0000)$ case we need branching rules for $(\lambda 000 \lambda)$ IR's of SU(6) to SU(3). That generating function has $1 + 9 - 3 = 7$ denominator factors [one independent SU(6) label, nine internal SU(6) labels, three internal SU(3) labels]. Substituting this into Eq. (7) gives a generating function with $1 + 7 - 1 = 7$ [1 and 7 are the numbers of denominators in the two generating functions, 1 is the number of SU(6) Dynkin labels to be eliminated]. Thus there are seven independent SO(3) scalars, and since there is one SO(3) Casimir, six missing label operators as required by the folk theorem.

Similarly, for the $(\lambda_1 \lambda_2 000)$ case we need branching rules for $SU(6) \supset SU(3)$ for the SU(6) IR's in the generating function (8); those SU(6) IR's have three independent IR labels $(\lambda_3 = 0, \ \lambda_1 + 2\lambda_2 = 2\lambda_4 + \lambda_5)$. Hence the $SU(6) \supset SU(3)$ generating function has $3 + 14 - 3 = 14$ denominators [3 SU(6) labels, 14 internal SU(6) labels, 3 internal SU(3) labels]. Substituting this into (8) gives a generating function with $4 + 14 - 3 = 15$ denominators [4 and 14 are the numbers of denominators in the two generating functions, 3 is the number of SU(6) labels to be eliminated]. Thus there are 15 independent SO(3) scalars and, since there is 1 SO(3) Casimir, 14 missing label operators, in agreement with the folk theorem.

Many other examples are found in Ref. 3, which deals with rank 2 groups and SU(4), and in Ref. 8, which deals with SO(7) and Sp(6).

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Indices of representations of simple superalgebras

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Indices and anomaly numbers for representations of basic classical Lie superalgebras are defined, and their explicit expressions are derived in terms of Kac–Dynkin labels. Useful properties of indices and anomalies are determined, and several examples are given. A similar analysis is made for superindices and superanomalies, and it is demonstrated how all these objects form a helpful tool in decomposing tensor products or in constructing branching rules for representations.

I. INTRODUCTION

The purpose of this paper is to extend the definition of the index of degree n, of a representation, well known in the case of semisimple Lie algebras, to representations of the simple superalgebras. It turns out that virtually all the valuable properties, which made the indices of representations so useful in computations, carry over to the new situation.

The index of degree 2 of a representation Λ of a semisimple Lie algebra L over $\mathbb{C}$ was originally defined and used by Dynkin[1] in classifying semisimple subalgebras of simple Lie algebras. It has proven to be useful in other applications.[2–5] In 1976 Dynkin's definition was reformulated and naturally extended[6] to include indices of degree >2. Subsequently, their applications became widespread. Here we single out only those papers where the indices (of any degree) are used in a new way or in a new form. Let us also mention that extensive tables of the values of indices are available[4,7,8]; in addition, with the other information provided in Ref. 8, the indices of any degree can easily be evaluated for all representations listed in that book.

In Ref. 9, indices were used to decompose plethysms. It turned out that general expressions for indices of plethysms could be found that are independent of the type of Lie algebra or representation on which the plethysms are based. Reference 10 contains a definition of the "anomaly numbers," well known in physics in a completely different way, which are so closely related to the indices of representations that it is appropriate to include them as well in the general notation of the index of a representation. The index of degree 2 is naturally related to the eigenvalue of the Casimir operator of the same degree. It is not so for higher indices as defined in Refs. 6 and 10; these are polynomials in the Casimir operators. Since it is sometimes advantageous to use the indices in conjunction with Casimir operators, a new definition of them was given[11–13] and extended to some of the applications. Then the index of degree k is automatically 0 if the Lie algebra does not have a Casimir operator of that degree. The anomaly cancellation conditions are naturally analyzed in terms of the indices of representations.[14]

Finally let us mention that recently the indices of representations were defined and their properties were described for representations of the Kac–Moody algebras.[15]

In the present paper we study indices and anomaly numbers for representations of the basic classical Lie superalgebras. The simple finite-dimensional Lie superalgebras were classified by Kac,[16] and some general theory of their representations was published by the same author.[17] The main difference with Lie algebras is that in general Lie superalgebras have so-called typical and atypical representations. Typical representations are irreducible highest weight representations, and their character χ_Λ is well known[17] in terms of the highest weight Λ. If Λ is "in atypical position" the corresponding irreducible highest weight module is atypical, and Kac's typical character formula[17] does not work. However, in that case the application of Kac's formula yields the character of an indecomposable representation. In this paper we make use of Kac's character formula in order to obtain an explicit expression for the index and the anomaly number. Hence, these expressions are valid for typical representations and for indecomposable representations, but not for atypical representations.

The structure of the paper is as follows: in Secs. II–IV we define indices and anomalies for representations of Lie superalgebras, investigate their properties, and determine their values. Section V contains some explicit examples. Superindices and superanomalies are analyzed in Sec. VI. In Sec. VII we demonstrate how the indices and anomalies are useful in constructing branching rules or in decomposing the tensor products of two representations. Finally, indices of plethysms are considered in Sec. VIII.

II. INDICES AND ANOMALIES FOR TYPICAL REPRESENTATIONS OF LIE SUPERALGEBRAS

For n an integer, we define the *index of order 2n* of a representation with highest weight Λ of a Lie superalgebra L as follows:

$$I_\Lambda^{(2n)} = \sum_\lambda (\lambda,\lambda)^n, \tag{2.1}$$

where the summation is over all weights λ (including multi-

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plicities) of the representation and $(\ ,\ )$ is some inner product on the weight space H^*. In order to have useful properties for the indices of Lie superalgebras, we shall have to make a special choice for this inner product. It is obvious that the bilinear form $\langle\lambda,\mu\rangle$ $(\lambda,\mu\in H^*)$ deduced from the invariant bilinear form on the Cartan subalgebra H of L does not satisfy our purposes. For instance, the existence of isotropic vectors[17] $\lambda\neq 0$ with $\langle\lambda,\lambda\rangle=0$ destroys the geometrical interpretation of indices and would make them useless for branching rules to Lie subalgebras. There is, however, a well-determined inner product $(\ ,\ )$ which satisfies all the properties needed and which is defined as follows. Let $L_{\bar 0}$ be the even part of the Lie superalgebra L, then[16]

$$L_{\bar 0}=G_a\oplus G_b\oplus G_c, \tag{2.2}$$

where every G_u is either a simple Lie algebra or the one-dimensional Lie algebra u(1), or else $G_u=0$. The explicit form of the simple components G_u of $L_{\bar 0}$ will be given in Secs. III and IV. Note that $G_c=0$ except for the Lie superalgebras spl(m,n) and $D(2,1;\alpha)$, where spl$(m,n)_{\bar 0}$ $=\mathrm{sl}(m)\oplus\mathrm{sl}(n)\oplus\mathrm{u}(1)$ and $D(2,1;\alpha)_{\bar 0}=A_1\oplus A_1\oplus A_1$. The decomposition (2.2) implies also that H and H^* can be written

$$H=H_a\oplus H_b\oplus H_c,\quad H^*=H_a^*\oplus H_b^*\oplus H_c^*, \tag{2.3}$$

where H_u is the Cartan subalgebra of G_u. Now, for every Lie algebra G_u the inner product $(\ ,\ )_u$ in the weight space H_u^* is well defined [with the normalization $(\alpha,\alpha)_u=2$ for α the longest root of G_u]. Hence, we define, for $\lambda=\lambda^a+\lambda^b+\lambda^c$ and $\mu=\mu^a+\mu^b+\mu^c$,

$$(\lambda,\mu)=(\lambda^a,\mu^a)_a+(\lambda^b,\mu^b)_b+(\lambda^c,\mu^c)_c. \tag{2.4}$$

This inner product will be described explicitly for all basic classical Lie superalgebras. The index can then be written as

$$I_\Lambda^{(2n)}=I_{\Lambda,a}^{(2n)}+I_{\Lambda,b}^{(2n)}+I_{\Lambda,c}^{(2n)}. \tag{2.5}$$

The properties of indices follow from the symmetry of weight diagrams of Lie superalgebras, which in their turn are derived from symmetries of weight diagrams of semisimple (or reductive) Lie algebras.[6] Let $\lambda\in H^*$ and λ_i^u $(i=1,\ldots,l_u)$ be the components of λ_u in an orthonormal basis with respect to $(\ ,\ )_u$; then the weight systems of representations of L satisfy

$$\sum_\lambda \lambda_i^u=0\quad[\text{for } G_u\neq\mathrm{u}(1)], \tag{2.6}$$

$$\sum_\lambda \lambda_i^u\lambda_j^{u'}=0\quad(\text{for } i\neq j). \tag{2.7}$$

This follows immediately from the fact that all weight systems of simple Lie algebras are rotationally symmetric to second order.[6] For $G_u=\mathrm{u}(1)$, (2.6) does not vanish, and hence representations of the Lie superalgebras spl(m,n) and $C(n)$ have a nonvanishing first-order *anomaly number* defined by

$$A_\Lambda=\sum_\lambda \lambda_1^u\quad[G_u=\mathrm{u}(1)], \tag{2.8}$$

where the summation is over all weights λ of the representation with highest weight Λ, and λ_1^u is the component of λ in the u(1)-direction.

The index has additivity properties similar to those of the dimension under reduction of a representation with highest weight Λ into representations with highest weights μ of some subalgebra L'. The only difference is the appearance of some coefficients ρ_u depending upon the projection of H^* into H'^* associated with the reduction $L\to L'$,

$$\sum_\mu I_\mu^{(2n)}=\sum_{u=a,b,c}\rho_u I_{\Lambda,u}^{(2n)}. \tag{2.9}$$

The coefficients ρ_u depend upon L and L', but not on Λ. Similarly, if the direct product of two representations (Λ_1) and (Λ_2) with dimensions N_1 and N_2, respectively, decomposes in representations with highest weight λ, then

$$\sum_\lambda I_\lambda^{(2)}=N_2 I_{\Lambda_1}^{(2)}+N_1 I_{\Lambda_2}^{(2)}+2A_{\Lambda_1}A_{\Lambda_2}. \tag{2.10}$$

III. THE INDEX FOR TYPE I LIE SUPERALGEBRAS

The type I Lie superalgebras are the series $A(m,n)$ and $C(n)$. They are characterized by the fact that their Lie algebraic part contains a one-dimensional center, namely $A(m-1,n-1)_{\bar 0}=\mathrm{spl}(m,n)_{\bar 0}=\mathrm{sl}(m)\oplus\mathrm{sl}(n)\oplus\mathrm{u}(1)$ (if $m\neq n$) and $C(n)_{\bar 0}=u(1)\oplus C_{n-1}$. Let Δ_0 and Δ_1 be the even and odd roots of L, and let a superscript $^+$ denote the positive roots in each set. We denote the Weyl group of L by W and the sign of $w\in W$ by $\epsilon(w)$. Then the character of a typical representation of L with highest weight Λ is given by[17]

$$\chi_\Lambda=B(\xi_\Lambda/\Delta), \tag{3.1}$$

with

$$B=\prod_{\beta\in\Delta_1^+}(e^{\beta\cdot\varphi/2}+e^{-\beta\cdot\varphi/2}), \tag{3.2}$$

$$\Delta=\prod_{\alpha\in\Delta_0^+}(e^{\alpha\cdot\varphi/2}-e^{-\alpha\cdot\varphi/2})=\sum_{w\in W}\epsilon(w)e^{w(\rho_0)\cdot\varphi}, \tag{3.3}$$

$$\xi_\Lambda=\sum_{w\in W}\epsilon(w)e^{w(\Lambda+\rho)\cdot\varphi}. \tag{3.4}$$

Here, $\rho=\rho_0-\rho_1$, where

$$\rho_0=\frac{1}{2}\sum_{\alpha\in\Delta_0^+}\alpha,\quad \rho_1=\frac{1}{2}\sum_{\beta\in\Delta_1^+}\beta. \tag{3.5}$$

In (3.2)–(3.4), we have introduced new formal variables $\varphi=(\varphi_1^a,\ldots,\varphi_{l_a}^a,\varphi_1^b,\ldots,\varphi_{l_b}^b,\varphi_1^c,\ldots,\varphi_{l_c}^c)$ which keep track of the components λ_i^u of a weight $\lambda=\lambda^a+\lambda^b+\lambda^c$ in the orthonormal basis, and $\lambda\cdot\varphi$ stands for

$$\sum_{u=a,b,c}\sum_{i=1}^{l_u}\lambda_i^u\varphi_i^u.$$

The character can also be written in the following form:

$$\chi_\Lambda=\sum_\lambda e^{\lambda\cdot\varphi}. \tag{3.6}$$

Then, it is clear that the second-order index is

$$I_\Lambda^{(2)}=\sum_{u=a,b,c}I_{\Lambda,u}^{(2)},\quad I_{\Lambda,u}^{(2)}=\sum_{i=1}^{l_u}\frac{\partial^2\chi_\Lambda}{(\partial\varphi_i^u)^2}\bigg|_{\varphi=0}; \tag{3.7}$$

similarly we have $\dim(\Lambda)=N_\Lambda=\chi_\Lambda|_{\varphi=0}$. From (3.1) one deduces that

$$I^{(2)}_{\Lambda,u} = \sum_i \frac{\partial^2 B}{(\partial\varphi^u_i)^2}\cdot\frac{\xi_\Lambda}{\Delta}\bigg|_{\varphi=0} + 2\sum_i \frac{\partial B}{\partial\varphi^u_i}\cdot\frac{\partial}{\partial\varphi^u_i}\left(\frac{\xi_\Lambda}{\Delta}\right)\bigg|_{\varphi=0} + B\sum_i \frac{\partial^2}{(\partial\varphi^u_i)^2}\left(\frac{\xi_\Lambda}{\Delta}\right)\bigg|_{\varphi=0}. \tag{3.8}$$

The first term reduces to

$$\sum_{\beta\in\Delta_1^+}\frac{1}{4}(\beta^u,\beta^u)B\cdot\frac{\xi_\Lambda}{\Delta}\bigg|_{\varphi=0} = N_\Lambda\cdot\sum_{\beta\in\Delta_1^+}\frac{1}{4}(\beta^u)^2, \tag{3.9}$$

where $(\beta^u)^2=(\beta^u,\beta^u)$. The second term vanishes, and the third term is equal to

$$\frac{B}{\Delta}\sum_i\frac{\partial^2\xi_\Lambda}{(\partial\varphi^u_i)^2}\bigg|_{\varphi=0} - \chi_\Lambda\cdot\frac{1}{\Delta}\sum_i\frac{\partial^2\Delta}{(\partial\varphi^u_i)^2}\bigg|_{\varphi=0} - 2\frac{B}{\Delta}\sum_i\frac{\partial}{\partial\varphi^u_i}\left(\frac{\xi_\Lambda}{\Delta}\right)\frac{\partial\Delta}{\partial\varphi^u_i}\bigg|_{\varphi=0}. \tag{3.10}$$

Making use of (3.3) and (3.4), one verifies that the first two terms in this expression yield

$$N_\Lambda[(\Lambda^u+\rho^u)^2-(\rho^u_0)^2]. \tag{3.11}$$

The last term in (3.10) is more elaborate to calculate. When $G_u=\mathrm{u}(1)$, this term clearly vanishes. For G_u a simple Lie algebra [$\neq\mathrm{u}(1)$], one can make use of properties of indices of simple Lie algebras.[6] Then this term is equal to

$$-[(n_u-l_u)/n_u]N_\Lambda[(\Lambda^u+\rho^u)^2-(\rho^u_0)^2]. \tag{3.12}$$

Here, $n_u=\dim(G_u)$ and $l_u=\operatorname{rank}G_u$. Hence, the final form of the index of a highest weight representation (Λ) is given by

$$I^{(2)}_\Lambda = N_\Lambda\cdot\sum_{u=a,b,c}\left\{\frac{1}{4}\sum_{\beta\in\Delta_1^+}(\beta^u)^2 + \frac{l_u}{n_u}[(\Lambda^u+\rho^u)^2-(\rho^u_0)^2]\right\} \tag{3.13}$$

$$= N_\Lambda\left\{\frac{1}{4}\sum_{\beta\in\Delta_1^+}\beta^2 + \sum_{u=a,b,c}\frac{l_u}{n_u}[(\Lambda^u+\rho^u)^2-(\rho^u_0)^2]\right\}, \tag{3.14}$$

where $\beta^2=(\beta,\beta)$. Note that the final form (3.13) or (3.14) includes the possibility $G_u=\mathrm{u}(1)$, in which case $n_u=l_u=1$.

For the first-order anomaly, defined in (2.8), one can also derive a simple expression in terms of the highest weight Λ. Let $G_c=\mathrm{u}(1)$, and let λ^c denote the component of a weight λ in the u(1)-direction. Then, using the same notation as before, one finds

$$A_\Lambda = \frac{\partial}{\partial\varphi^c}(\chi_\Lambda)\bigg|_{\varphi=0}. \tag{3.15}$$

Making use of the explicit character formula given by (3.1), we find

$$A_\Lambda = N_\Lambda(\Lambda^c+\rho^c). \tag{3.16}$$

A. The index and anomaly for $A(m-1,n-1)=\mathrm{spl}(m,n)$ $(m\neq n)$

The positive roots of spl(m,n) are given by[17]

$$\Delta_0^+ = \{\epsilon_i-\epsilon_j\ (1\leqslant i<j\leqslant m),\ \delta_i-\delta_j\ (1\leqslant i<j\leqslant n)\}, \tag{3.17}$$

$$\Delta_1^+ = \{\epsilon_i-\delta_j\ (1\leqslant i\leqslant m,\ 1\leqslant j\leqslant n)\}. \tag{3.18}$$

The even part of spl(m,n) is $\mathrm{sl}(m)\oplus\mathrm{sl}(n)\oplus\mathrm{u}(1)$. The Cartan subalgebra of sl(m) is spanned by $\epsilon_1-\epsilon_2,\ldots,\epsilon_{m-1}-\epsilon_m$, or similarly by the dependent elements ϵ_i $(i=1,\ldots,m)$ with $\Sigma_{i=1}^m\epsilon_i=0$. The inner product $(\ ,\ )_a$ is determined by

$$(\epsilon_i,\epsilon_j)_a=\delta_{ij}-1/m. \tag{3.19}$$

The same holds for sl(n),

$$(\delta_i,\delta_j)_b=\delta_{ij}-1/n. \tag{3.20}$$

Finally, one can verify that the basis vector in the u(1) direction is given by

$$\eta=\frac{1}{m}\left(\sum_{i=1}^m\epsilon_i\right)-\frac{1}{n}\left(\sum_{i=1}^n\delta_i\right). \tag{3.21}$$

Let $\mu\in H^*$, say

$$\mu=\sum_{i=1}^m\mu_i\epsilon_i+\sum_{i=1}^n\mu_{m+i}\delta_i. \tag{3.22}$$

The μ_i's are determined "up to a constant term" since

$$\sum_{i=1}^m\epsilon_i-\sum_{i=1}^n\delta_i=0 \tag{3.23}$$

in H^*. The Kac–Dynkin labels for μ are equal to

$$a_i=\mu_i-\mu_{i+1}\quad(i=1,\ldots,m-1,m+1,\ldots,m+n),\qquad a_m=\mu_m+\mu_{m+1}. \tag{3.24}$$

Then we have

$$(\mu,\mu)_a=\left(\sum_{i=1}^m\mu_i\epsilon_i,\sum_{j=1}^m\mu_j\epsilon_j\right)_a = \frac{1}{m}\sum_{i<j}(\mu_i-\mu_j)^2\quad(i,j=1,\ldots,m),$$
$$(\mu,\mu)_b=\frac{1}{n}\sum_{i<j}(\mu_{m+i}-\mu_{m+j})^2\quad(i,j=1,\ldots,n),$$
$$(\mu\mu)_c=\left(\frac{n}{n-m}\sum_{i=1}^m\mu_i+\frac{m}{n-m}\sum_{i=1}^n\mu_{m+i}\right)^2. \tag{3.25}$$

Obviously, all values in (3.25) are invariant under replacement of μ by $\mu+z(\Sigma\epsilon_i-\Sigma\delta_j)$, $z\in\mathbb{C}$.

Using these properties, one obtains

$$\sum_{\beta\in\Delta_1^+}\beta^2=3mn-m-n. \tag{3.26}$$

Let Λ be the highest weight of a typical representation with Kac–Dynkin labels $(a_1,\ldots,a_{m+n-1})$. We define new labels l_i by means of

$$l_i = \left(\sum_{j=i}^{m} a_j - \sum_{j=1}^{n-1} a_{m+j}\right) + \frac{m-n+1}{2} - i \quad (i = 1,\ldots,m),$$

$$l_{m+i} = \left(\sum_{j=i}^{n-1} a_{m+i}\right) + \frac{m+n+1}{2} - i \quad (i = 1,\ldots,n-1), \tag{3.27}$$

$$l_{m+n} = \frac{m-n+1}{2}.$$

Then one finds

$$(\Lambda^a + \rho^a)^2 = \frac{1}{m}\sum_{i<j=1}^{m} (l_i - l_j)^2,$$

$$(\Lambda^b + \rho^b)^2 = \frac{1}{n}\sum_{i<j=1}^{n} (l_{m+i} - l_{m+j})^2, \tag{3.28}$$

$$(\Lambda^c + \rho^c)^2 = \left(\frac{n}{n-m}\sum_{i=1}^{m} l_i + \frac{m}{n-m}\sum_{i=1}^{n} l_{m+i}\right)^2.$$

Therefore, the index is given by

$$I_\Lambda^{(2)} = N_\Lambda \left\{ \frac{1}{4}(3mn - m - n) + \frac{1}{m(m+1)}\left[\sum_{i<j=1}^{m} (l_i - l_j)^2 - \frac{1}{12}m^2(m+1)(m-1)\right] \right.$$

$$\left. + \frac{1}{n(n+1)}\left[\sum_{i<j=1}^{n} (l_{m+i} - l_{m+j})^2 - \frac{1}{12}n^2(n+1)(n-1)\right] + \left(\frac{n}{n-m}\sum_{i=1}^{m} l_i + \frac{m}{n-m}\sum_{i=1}^{n} l_{m+i}\right)^2 \right\}. \tag{3.29}$$

The dimension N_Λ has been determined by Kac for all basic classical Lie superalgebras.

Also for the anomaly number of a typical representation of spl(m,n), one finds a simple expression,

$$A_\Lambda = N_\Lambda \left(\frac{n}{n-m}\sum_{i=1}^{m} l_i + \frac{m}{n-m}\sum_{i=1}^{n} l_{m+i}\right). \tag{3.30}$$

B. Index and anomaly for $C(n)$=osp(2,2n–2) (n>2)

The roots of $C(n)$ are given by[17]

$$\Delta_0^+ = \{\delta_i - \delta_j, \delta_i + \delta_j, 2\delta_i\} \quad (1 \leqslant i < j \leqslant n-1),$$

$$\Delta_1^+ = \{\epsilon - \delta_i, \epsilon + \delta_i\}. \tag{3.31}$$

Clearly, ϵ is the basis vector in the u(1)-direction. The inner product on H^* is determined by

$$(\epsilon,\epsilon)_a = 1, \quad (\delta_i,\delta_j)_b = \tfrac{1}{2}\delta_{ij}. \tag{3.32}$$

Then, we find that

$$\sum_{\beta\in\Delta_1^+} \beta^2 = 3(n-1). \tag{3.33}$$

For a typical highest weight representation (Λ) with Kac–Dynkin labels $(a_1,\ldots,a_n)$, we introduce the following labels l_i:

$$l_1 = a_1,$$

$$l_{1+i} = \left(\sum_{k=1+i}^{n} a_k\right) + n - i \quad (i = 1,\ldots,n-1). \tag{3.34}$$

Consequently,

$$I_\Lambda = N_\Lambda \left\{ \frac{3}{4}(n-1) + \frac{1}{2(2n-1)} \right.$$

$$\left. \times \sum_{i=1}^{n-1} [l_{1+i}^2 - (l_{1+i}^0)^2] + (l_1 + 1 - n)^2 \right\}. \tag{3.35}$$

Here, l_i^0 are the labels l_i with all a_j's replaced by 0.

The anomaly number is determined by means of formula (3.16)

$$A_\Lambda = N_\Lambda (a_1 - n + 1). \tag{3.36}$$

IV. THE INDEX FOR TYPE II LIE SUPERALGEBRAS

The even subspaces of type II Lie superalgebras are semisimple Lie algebras. The lack of a u(1) part makes the situation slightly simpler. On the other hand, calculations are now complicated by the fact that $\Lambda + \rho$ is not always an integral weight for the semisimple Lie algebra $L_{\bar 0}$. Let $L_{\bar 0} = \oplus_{u=a,b,c} G_u$, then one finds that the index of a typical highest weight representation (Λ) is given by

$$I_\Lambda^{(2)} = N_\Lambda \left\{ \frac{1}{4}\sum_{\beta\in\Delta_1^+} \beta^2 + \sum_u \frac{l_u}{n_u}[(\Lambda^u + \rho^u)^2 - (\rho_0^u)^2] \right\}, \tag{4.1}$$

where $l_u = \text{rank } G_u$, $n_u = \dim G_u$, and $(\lambda^u)^2 = (\lambda^u, \lambda^u)_u$ is the square length of the projection of λ onto H_u^*.

A. $B(m,n)$=osp(2m+1,2n) (m>0,n>0)

The roots of $B(m,n)$ are given by

$$\Delta_0^+ = \{\delta_i - \delta_j, \delta_i + \delta_j, 2\delta_i \ (1 \leqslant i < j \leqslant n);$$

$$\epsilon_i - \epsilon_j, \epsilon_i + \epsilon_j, \epsilon_i \quad (1 \leqslant i < j \leqslant m)\}, \tag{4.2}$$

$$\Delta_1^+ = \{\delta_i - \epsilon_j, \delta_i + \epsilon_j, \delta_i\}. \tag{4.3}$$

Here, $L_{\bar 0} = B_m \oplus C_n$, and hence the inner product on H^* is given by

$$(\epsilon_i,\epsilon_j) = \delta_{ij}, \quad (\epsilon_i,\delta_j) = 0, \quad (\delta_i,\delta_j) = \tfrac{1}{2}\delta_{ij}, \tag{4.4}$$

for $m > 1$. When $m = 1$, the longest root of B_1 is ϵ_1, and we have to choose a different normalization. It is easy to see that

$$\sum_{\beta\in\Delta_1^+} \beta^2 = 3mn + \tfrac{1}{2}n. \tag{4.5}$$

Let λ be the highest weight of a typical irrep, characterized

by the Kac–Dynkin labels $(a_1,...,a_{m+n})$. We define the labels l_i by means of

$$l_i = \left(\sum_{k=i}^{m-1} a_{n+k}\right) + \frac{1}{2}a_{n+m} + m - i + \frac{1}{2} \quad (i=1,...,m),$$

$$l_{m+i} = \left(\sum_{k=i}^{n} a_k\right) - \left(\sum_{k=1}^{m-1} a_{n+k}\right) - \frac{1}{2}a_{n+m} + n - i + 1 \quad (i=1,...,n). \tag{4.6}$$

Then

$$[(\Lambda^a+\rho^a)^2 - (\rho_0^a)^2] = \sum_{i=1}^{m} [l_i^2 - (l_i^0)^2],$$

$$[(\Lambda^b+\rho^b)^2 - (\rho_0^b)^2] = \frac{1}{2}\sum_{i=1}^{n}\left[\left(l_i - m - \frac{1}{2}\right)^2 - (l_i^0)^2\right], \tag{4.7}$$

where l_i^0 is again l_i with all labels $a_j = 0$. With $l_a/n_a = (2m+1)^{-1}$ and $l_b/n_b = (2n+1)^{-1}$, we have everything needed to calculate $I_\Lambda^{(2)}$ for $B(m,n)$ by means of (4.1).

When $m=1$, the choice of the linear product is different, namely,

$$(\epsilon_1,\epsilon_1) = 2, \quad (\epsilon_1,\delta_j) = 0, \quad (\delta_i,\delta_j) = \tfrac{1}{2}\delta_{ij}, \tag{4.8}$$

and hence

$$\sum_{\beta\in\Delta_1^+} \beta^2 = \frac{11n}{2}. \tag{4.9}$$

Using the same labels l_i as in (4.6), we find now

$$[(\Lambda^a+\rho^a)^2 - (\rho_0^a)^2] = 2[l_1^2 - (l_1^0)^2]. \tag{4.10}$$

The other contributions in $I_\Lambda^{(2)}$ are the same as for $m>1$.

B. $B(0,n)=\mathrm{osp}(1,2n)$ $(n>0)$

The even roots of $B(0,n)$ are those of C_n, and the odd roots are given by

$$\Delta_1^+ = \{\delta_i\} \quad (i=1,...,n). \tag{4.11}$$

Since $L_{\bar 0} = C_n$, the inner product is

$$(\delta_i,\delta_j) = \tfrac{1}{2}\delta_{ij}. \tag{4.12}$$

Then, one finds

$$\sum_{\beta\in\Delta_1^+} \beta^2 = \frac{1}{2}n. \tag{4.13}$$

Introducing the labels l_i $(i=1,...,n)$ in terms of the Kac–Dynkin labels $(a_1,...,a_n)$ of an irrep with highest weight Λ by

$$l_i = \sum_{k=i}^{n-1} a_k + \frac{1}{2}a_n + n - i + 1 \quad (i=1,...,n), \tag{4.14}$$

one can verify that

$$I_\Lambda^{(2)} = N_\Lambda\left\{\frac{1}{8}n + \frac{1}{2(2n+1)}\sum_{i=1}^{n}\left[\left(l_i - \frac{1}{2}\right)^2 - (l_i^0)^2\right]\right\}. \tag{4.15}$$

C. $D(m,n)=\mathrm{osp}(2m,2n)$ $(m>1)$

The roots of $D(m,n)$ can be given in the following form:

$$\Delta_0^+ = \{\delta_i - \delta_j, \delta_i + \delta_j, 2\delta_i \ (1\leqslant i<j\leqslant n); \ \epsilon_i - \epsilon_j, \epsilon_i + \epsilon_j \ (1\leqslant i<j\leqslant m)\}, \tag{4.16}$$

$$\Delta_1^+ = \{\delta_i - \epsilon_j, \delta_i + \epsilon_j\}. \tag{4.17}$$

The inner product on the Cartan subalgebra of $L_{\bar 0} = D_m \oplus C_n$ is determined by

$$(\epsilon_i,\epsilon_j) = \delta_{ij}, \quad (\epsilon_i,\epsilon_j) = 0, \quad (\delta_i,\delta_j) = \tfrac{1}{2}\delta_{ij}. \tag{4.18}$$

It follows that

$$\sum_{\beta\in\Delta_1^+} \beta^2 = 3mn. \tag{4.19}$$

For a typical irrep with highest weight Λ and corresponding Kac–Dynkin labels $(a_1,...,a_{m+n})$, we introduce the new labels l_i,

$$l_i = \left(\sum_{k=i}^{m-2} a_{n+k}\right) + \frac{1}{2}(a_{n+m-1} + a_{n+m}) + m - i \quad (i=1,...,m-1),$$

$$l_m = \tfrac{1}{2}(-a_{n+m-1} + a_{n+m}), \tag{4.20}$$

$$l_{m+i} = \left(\sum_{k=i}^{n} a_k\right) - \left(\sum_{k=1}^{m-2} a_{n+k}\right) - \frac{1}{2}(a_{n+m-1} + a_{n+m}) + n - i + 1 \quad (i=1,...,n).$$

Then, one has

$$[(\Lambda^a+\rho^a)^2 - (\rho_0^a)^2] = \sum_{i=1}^{m} [l_i^2 - (l_i^0)^2],$$

$$[(\Lambda^b+\rho^b)^2 - (\rho_0^b)^2] = \frac{1}{2}\sum_{i=1}^{n} [(l_{m+i} - m)^2 - (l_{m+i}^0)^2]. \tag{4.21}$$

With $l_a/n_a = (2m-1)^{-1}$ and $l_b/n_b = (2n+1)^{-1}$, these values determine $I_\Lambda^{(2)}$ completely.

D. $D(2,1;\alpha)$

The even positive roots of $D(2,1;\alpha)$ are given by $2\epsilon_i$ $(i=1,2,3)$, and the odd positive roots by[18]

$$\Delta_1^+ = \{\epsilon_1 - \epsilon_2 - \epsilon_3, \epsilon_1 - \epsilon_2 + \epsilon_3, \epsilon_1 + \epsilon_2 - \epsilon_3, \epsilon_1 + \epsilon_2 + \epsilon_3\}. \tag{4.22}$$

The inner product on H^* is determined by

$$(\epsilon_i,\epsilon_j) = \tfrac{1}{2}\delta_{ij}. \tag{4.23}$$

Hence

$$\sum_{\beta\in\Delta_1^+} \beta^2 = 6. \tag{4.24}$$

We introduce the labels l_i for a highest weight irrep (Λ) in terms of the Kac–Dynkin labels a_i by

$$l_1 = [1/(1+\alpha)](2a_1 - a_2 - \alpha a_3), \quad l_2 = a_2, \quad l_3 = a_3. \tag{4.25}$$

Then, one finds

$$I_\Lambda^{(2)} = N_\Lambda \cdot \tfrac{1}{6}(l_1^2 + l_2^2 + l_3^2 - 2l_1 + 2l_2 + 2l_3 + 9). \tag{4.26}$$

E. $G(3)$

The roots of $G(3)$ are expressed[17] in terms of δ and ϵ_i $(i=1,2,3)$ satisfying $\epsilon_1 + \epsilon_2 + \epsilon_3 = 0$,

$$\Delta_0^+ = \{\epsilon_2,\epsilon_3-\epsilon_2,\epsilon_3,-\epsilon_1,\epsilon_2-\epsilon_1,\epsilon_3-\epsilon_1;2\delta\}, \quad (4.27)$$

$$\Delta_1^+ = \{\delta+\epsilon_i,\delta-\epsilon_i,\delta\} \quad (i=1,2,3), \quad (4.28)$$

and the inner product on H^* reads

$$(\delta,\delta)=\tfrac{1}{2}, \quad (\delta,\epsilon)=0, \quad (\epsilon_i,\epsilon_j)=\delta_{ij}-\tfrac{1}{3}. \quad (4.29)$$

For a highest weight representation (Λ) with Kac–Dynkin labels (a_i), $\Lambda = l_1\delta + l_2\epsilon_1 + l_3\epsilon_2$, where

$$l_1=\tfrac{1}{2}(a_1-2a_2-3a_3), \quad l_2=-a_2-2a_3, \quad l_3=-a_3. \quad (4.30)$$

Then, (4.1) gives rise to

$$I_\Lambda^{(2)} = N_\Lambda\{\tfrac{1}{4}+\tfrac{1}{6}(l_1^2-5l_1) + \tfrac{2}{21}(l_2^2-l_2l_3+l_3^2-3l_2+3l_3-4)\}. \quad (4.31)$$

F. $F(4)$

The positive roots of $F(4)$ are[17]

$$\Delta_0^+ = \{\epsilon_j-\epsilon_k,\epsilon_j+\epsilon_k,\epsilon_j,2\delta\} \quad (1\leqslant j<k\leqslant 3), \quad (4.32)$$

$$\Delta_1^+ = \{\delta+\tfrac{1}{2}(\pm\epsilon_1\pm\epsilon_2\pm\epsilon_3)\} \quad \text{(independent } \pm \text{ signs)}. \quad (4.33)$$

The inner product is determined by

$$(\delta,\delta)=\tfrac{1}{2}, \quad (\delta,\epsilon_i)=0, \quad (\epsilon_i,\epsilon_j)=\delta_{ij}. \quad (4.34)$$

Expressing the labels l_i in terms of the Kac–Dynkin labels (a_i) for an irrep with highest weight

$$\Lambda = l_1\delta + \sum_{i=1}^{3} l_{1+i}\epsilon_i,$$

one finds

$$l_1=\tfrac{1}{3}(2a_1-3a_2-4a_3-2a_4),$$

$$l_2=a_4+a_3+\tfrac{1}{2}a_2, \quad l_3=a_3+\tfrac{1}{2}a_2, \quad l_4=\tfrac{1}{2}a_2. \quad (4.35)$$

Then, the index reads

$$I_\Lambda^{(2)} = N_\Lambda\{\tfrac{1}{6}(l_1^2-6l_1)+\tfrac{1}{7}(l_2^2+5l_2 + l_3^2+3l_3+l_4^2+l_4)+\tfrac{17}{3}\}. \quad (4.36)$$

V. EXAMPLES

A. $A(1,0)=\mathrm{spl}(2,1)$

Let (a_1,a_2) be the Kac–Dynkin labels of a typical representation of spl(2,1): $\overset{a_1}{\circ}\!\!-\!\!\otimes\overset{a_2}{}$. Then $\Lambda=(a_1+a_2)\epsilon_1+a_2\epsilon_2$, and the u(1)-label of Λ is given by $k=-a_1-2a_2$. The corresponding sl(2) label is $j=a_1$. Applying (3.29) one finds, with $N_\Lambda=4(a_1+1)$, that

$$I_\Lambda^{(2)} = 4(a_1+1)\{\tfrac{3}{4}+\tfrac{1}{6}(a_1^2+2a_1)+(a_1+2a_2+1)^2\}, \quad (5.1)$$

or, expressed in the more conventional labels[19] $(k;j)$,

$$I_\Lambda^{(2)} = 4(j+1)[\tfrac{1}{6}(j^2+2j)+k^2-2k+\tfrac{7}{4}]. \quad (5.2)$$

B. $C(2)=\mathrm{osp}(2,2)$

For a representation with Kac–Dynkin labels

$\overset{a_1}{\otimes}\!\!\Longleftarrow\!\!\overset{a_2}{\circ}$,

the highest weight Λ is equal to $a_1\epsilon+a_2\delta_1$, or, more conveniently[19] $k\epsilon+j\delta_1$, where $(k;j)=(a_1;a_2)$. Since $N_\Lambda=4(j+1)$, (3.35) gives immediately

$$I_\Lambda^{(2)} = 4(j+1)[\tfrac{1}{6}(j^2+2j)+k^2-2k+\tfrac{7}{4}]. \quad (5.3)$$

This is exactly the same expression as (5.2). Clearly, this follows from the fact that osp(2,2) = spl(2,1). In this case, also the expression (3.36) for the anomaly becomes very simple,

$$A_\Lambda = 4(j+1)(k-1). \quad (5.4)$$

C. $B(0,1)=\mathrm{osp}(1,2)$

Let $s=2a$ be twice the Kac–Dynkin label. Then s is always an integer, and since $N_\Lambda=2s+1$, (4.15) implies

$$I_\Lambda^{(2)} = \tfrac{1}{6}s(s+1)(2s+1). \quad (5.5)$$

Obviously, since the weights of the irrep are given by $k\delta$ $(k=-s,-s+1,\ldots,+s)$ and $(\delta,\delta)=\frac{1}{2}$, the above expression can also be easily obtained from the definition of the index.

D. $B(1,1)=\mathrm{osp}(3,2)$

Let Λ be a typical irrep with Kac–Dynkin labels

$\overset{a_1}{\otimes}\!\!\Longrightarrow\!\!\overset{a_2}{\circ}$.

Then $\Lambda=\frac{1}{2}a_2\epsilon_1+(a_1-\frac{1}{2}a_2)\delta_1$. In terms of the labels $(q;p)$ introduced previously (see Ref. 19) we have $\Lambda=\frac{1}{2}p\epsilon_1+q\delta_1$. Since $N_\Lambda=4(2q-1)(p+1)$, one finds from (4.7), (4.9), and (4.10),

$$I_\Lambda^{(2)} = \tfrac{2}{3}(2q-1)(p+1)[p^2+2p+q^2-q+\tfrac{15}{2}]. \quad (5.6)$$

E. $D(2,1)=\mathrm{osp}(4,2)=D(2,1;1)$

For a representation with Kac–Dynkin labels (a_1,a_2,a_3), the highest weight is given by[19] $\Lambda=p\epsilon_1+q\epsilon_2+r\epsilon_3$ with $p=(2a_1-a_2-a_3)/2$, $q=a_2$, $r=a_3$. The dimension of this representation is $16(p-1)(q+1)(r+1)$, hence (4.19)–(4.21) leads to

$$I_\Lambda^{(2)} = \tfrac{8}{3}(p-1)(q+1)(r+1) \times[p^2-2p+q^2+2q+r^2+2r+9]. \quad (5.7)$$

VI. THE SUPERINDEX AND SUPERANOMALY

For n an integer, we define the *superindex* of order $(2n)$ of a representation with highest weight Λ of a Lie superalgebra L by

$$S_\Lambda^{(2n)} = \sum_\lambda (-1)^{\sigma(\lambda)}(\lambda,\lambda)^n, \quad (6.1)$$

where $(\ ,\ )$ is the inner product on H^* introduced previously, and $\sigma(\lambda)$ is the degree of the weight λ: $\sigma(\lambda)\in\mathbb{Z}_2$. Note that the zero-order superindex is equal to the superdimension N_Λ^S. The *superanomaly* A_Λ^S is defined in a similar way. Let λ^c denote the component of a weight λ in the u(1)-direction. Then

$$A_\Lambda^S = \sum_\lambda (-1)^{\sigma(\lambda)}\lambda^c. \quad (6.2)$$

The superindex has properties similar to those of the index. If a representation with highest weight Λ decomposes into representations with highest weights μ of some subalgebra, then

$$\sum_{\mu} S_{\mu}^{(2n)} = \sum_{u=a,b,c} \rho_u S_{\Lambda,u}^{(2n)}, \tag{6.3}$$

where the ρ_u are the same as in (2.9). And if the direct product of two representations (Λ_1) and (Λ_2) with superdimensions N_1^S and N_2^S, respectively, decomposes into representations with highest weights λ, then

$$\sum_{\lambda} S_{\lambda}^{(2)} = N_2^S S_{\Lambda_1}^{(2)} + N_1^S S_{\Lambda_2}^{(2)} + 2A_{\Lambda_1}^S A_{\Lambda_2}^S. \tag{6.4}$$

Remember that for a typical representation (Λ) of any basic classical Lie superalgebra L different from $B(0,n)$ one has $N_{\Lambda}^S = 0$.

The superindex can be expressed in terms of the supercharacter χ_{Λ}^S of a representation. Kac[17] has given a general formula for the supercharacter of a typical representation,

$$\chi_{\Lambda}^S = B^S(\xi_{\Lambda}^S/\Lambda) \tag{6.5}$$

with

$$B^S = \prod_{\beta\in\Delta_1^+} (e^{\beta\cdot\varphi/2} - e^{-\beta\cdot\varphi/2}), \tag{6.6}$$

$$\xi_{\Lambda}^S = \sum_{w\in W} \epsilon'(w) e^{w(\Lambda+\rho)\cdot\varphi}, \tag{6.7}$$

and Δ is the same as in (3.3). In order to define $\epsilon'(w)$, let

$$\overline{\Delta}_0^+ = \{\alpha\in\Delta_0^+ \mid (\alpha/2)\notin\Delta_1^+\}. \tag{6.8}$$

Then $\epsilon'(w)$ is $+1$ (resp. -1), if the number of reflections with respect to the roots of $\overline{\Delta}_0^+$ in the expression of w is even (resp. odd). The supercharacter can also be written in the following form:

$$\chi_{\Lambda}^S = \sum_{\lambda \text{ even}} e^{\lambda\cdot\varphi} - \sum_{\lambda \text{ odd}} e^{\lambda\cdot\varphi}. \tag{6.9}$$

Hence, $S_{\Lambda}^{(2)} = \Sigma_u S_{\Lambda,u}^{(2)}$ with

$$S_{\Lambda,u}^{(2)} = \sum_{i=1}^{l_u} \frac{\partial^2 \chi_{\Lambda}^S}{(\partial\varphi_i^u)^2}\bigg|_{\varphi=0}. \tag{6.10}$$

From the supercharacter formula one can, at least in some cases, derive a general expression for the superindex. First, let $L \neq B(m,n)$ or $G(3)$. Then[17] $\overline{\Delta}_0^+ = \Delta_0^+$, and hence $\epsilon'(w) = \epsilon(w)$, or $\xi_{\Lambda}^S = \xi_{\Lambda}$. Now, one can do a calculation similar to that in Sec. III. All terms that become proportional to the superdimension vanish, since $N_{\Lambda}^S = 0$ for typical representations. Then, it is easy to check that for $L \neq B(m,n)$ or $G(3)$,

$$S_{\Lambda}^{(2)} = 0 \quad \text{for } \#\Delta_1^+ > 2. \tag{6.11}$$

The last condition follows from the explicit form of $\Sigma_i(\partial^2 B/\partial\varphi_i^2)$ and the fact that B contains exactly $\#\Delta_1^+$ factors.

Due to the appearance of $\epsilon'(w)$, we have not been able to derive a general expression for $S_{\Lambda}^{(2)}$ in the case of $L = B(m,n)$ or $G(3)$.

Also the superanomaly can be evaluated. Now $L = A(m,n)$ or $C(n)$, since the superanomaly vanishes otherwise, and therefore $\chi_{\Lambda}^S = B^S\xi_{\Lambda}/\Delta$. Let λ^c denote the component of a weight λ in the u(1)-direction; then

$$A_{\Lambda}^S = \frac{\partial}{\partial\varphi^c}(\chi_{\Lambda}^S)\bigg|_{\varphi=0}. \tag{6.12}$$

Explicit calculations show that A_{Λ}^S is proportional to N_{Λ}^S, hence

$$A_{\Lambda}^S = 0 \tag{6.13}$$

for all typical representations of all Lie superalgebras.

Finally, we shall determine some explicit expressions for superindices of certain Lie superalgebras. For the examples considered here, the structure of the representations is well known,[19] and we could calculate the superindex making use of the decomposition into irreps of the even part $L_{\bar{0}}$. The notation is the same as introduced previously (see Sec. V). The appearance of a $\pm$ sign should be interpreted as follows: the upper sign corresponds to the value of the superindex with the highest weight an even weight, the lower sign with the highest weight an odd weight.

1. spl(2,1)=osp(2,2)

spl(2,1) is a superalgebra with $\#\Delta_1^+ = 2$, so $S_{\Lambda}^{(2)}$ need not be 0. Indeed we find

$$S_{\Lambda}^{(2)} = \pm(j+1). \tag{6.14}$$

2. osp(1,2)=B(0,1)

$$S_{\Lambda}^{(2)} = \pm\tfrac{1}{2}s(s+1). \tag{6.15}$$

3. osp(3,2)=B(1,1)

$$S_{\Lambda}^{(2)} = \mp 3(p+1). \tag{6.16}$$

4. osp(4,2)=D(2,1)

$$S_{\Lambda}^{(2)} = 0. \tag{6.17}$$

VII. SOME APPLICATIONS

Let us first illustrate how the indices can be used to verify branching rules. Let $L = D(2,1)$ and consider its principal[20] $B(0,1)$ subalgebra. One way to determine how a representation $(p;q;r)$ of $D(2,1)$ decomposes into irreps (s) of $B(0,1)$ is to construct the weight diagram of $(p;q;r)$ explicitly and then deduce the subalgebra contents by projecting on the subalgebra weight space. Using this method, we have found, for instance,

$$(3;1;0) \to (5) + 2(4) + 2(3) + 3(2) + 2(1), \tag{7.1}$$

where the number in front of (s) denotes the multiplicity of the irrep (s). This decomposition can be verified in three ways, namely by using the dimensions, indices (2.9), and superindices (6.3):

$$\text{dimensions:} \quad 64 = 11 + 2\times 9 + 2\times 7 + 3\times 5 + 2\times 3, \tag{7.2}$$

$$\text{indices:} \quad 160 = 55 + 2\times 30 + 2\times 14 + 3\times 5 + 2\times 1, \tag{7.3}$$

$$\text{superindices:} \quad 0 = -15 + 2\times 10 - 2\times 6 + 3\times 3 - 2\times 1. \tag{7.4}$$

Since $B(0,1)$ is the principal subalgebra of $D(2,1)$, one has to take $\rho_a = \rho_b = \rho_c = 1$ in (2.9) and (6.3). Then they give rise to (7.3) and (7.4). Note that in many cases the relations arising from dimensions, indices, and superindices enable us to find the decomposition of representations. As an example,

consider $(p;q;r) = (2;1;0)$. Since $B(0,1)$ is a principal subalgebra, the highest s-value is $p+q+r+1$, which is 4, and it occurs with multiplicity 1. Hence, the decomposition must be of the form

$$(2;1;0) \to (4) + a(3) + b(2) + c(1) + d(0). \tag{7.5}$$

Then, dimensions, indices, and superindices give rise to the following three relations, respectively:

$$7a + 5b + 3c + d = 23, \tag{7.6}$$

$$14a + 5b + c = 34, \tag{7.7}$$

$$6a - 3b + c = 10. \tag{7.8}$$

Moreover, we have the condition that a, b, c, and d must be non-negative integers. Hence, it follows from (7.7) that a can only be 0, 1, or 2. For $a=0$, we find $(b,c,d) = (3,19,-49)$; for $a=1$, $(b,c,d) = (2,10,-24)$, and for $a=2$ one obtains $(b,c,d) = (1,1,1)$, which is the only acceptable solution. Consequently, the decomposition reads

$$(2;1;0) \to (4) + 2(3) + (2) + (1) + (0). \tag{7.9}$$

As a second example, we shall illustrate how the indices and superindices can be used in order to verify—or sometimes determine—the decomposition of the tensor product of two representations. Consider the case of $L = C(2)$ with Λ_1: $(k;j) = (1;2)$ and Λ_2: $(k;j) = (1;3)$. Then $N_{\Lambda_1} = 12$, $I^{(2)}_{\Lambda_1} = 25$, $N_{\Lambda_2} = 16$, $I^{(2)}_{\Lambda_2} = 52$, and $A_{\Lambda_1} = A_{\Lambda_2} = 0$. Hence

$$N_{\Lambda_2} I^{(2)}_{\Lambda_1} + N_{\Lambda_1} I^{(2)}_{\Lambda_2} + 2A_{\Lambda_1} A_{\Lambda_2} = 1024. \tag{7.10}$$

Now, from weight space techniques one can calculate the following decomposition of the tensor product:

$$(1;2) \otimes (1;3) \to (2;5) + (2;3) + (2;1) + (1;6) + 2(1;4) + 2(1;2) + (1;0) + (0;5) + (0;3) + (0;1). \tag{7.11}$$

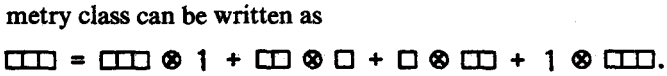
Then, using (5.3), it is easy to see that the indices in the rhs of (7.11) are given by

$$182 + 68 + 18 + 245 + 2\times 95 + 2\times 25 + 3 + 182 + 68 + 18 = 1024.$$

It turns out that the indices provide us with a very useful and nontrivial check for the decomposition of the tensor product of two representations.

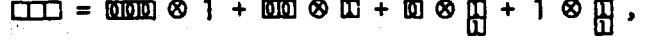
VIII. (SUPER)INDICES AND (SUPER)ANOMALIES FOR PLETHYSMS

In this final section we present some formulas for (super)indices and (super)anomalies of plethysms for Lie superalgebras. A plethysm for a Lie algebra is the component of the direct product of n copies of some representation ρ whose permutation symmetry is described by a Young tableau.[9] For Lie superalgebras, a representation ρ contains both even and odd weights. A supersymmetry class of n copies of ρ is then defined by taking the corresponding class for the even weights and the conjugate class for the odd weights. For example, consider first the symmetry class determined by the Young tableau $\square\square\square$. If we divide the original set of weights into two disjoint sets of weights, this symmetry class can be written as



(8.1)

Hence, if we split even and odd weights, we obtain for the supersymmetry class



(8.2)

where the boxes in the rhs of (8.2) have been labeled by 0 or 1 when they refer to even or odd weights, respectively.

We denote the representation ρ on which a plethysm is based by a single box $\square$. This representation ρ may be reducible, irreducible, indecomposable, typical, or atypical. Its dimension is N, its superdimension N_S. Furthermore, its second-order index is $I_\square$, its second-order superindex is $S_\square$, its first-order anomaly is $A_\square$, and its first-order superanomaly is $A^S_\square$.

The index for a supersymmetry class can now be determined by calculating the indices for the corresponding symmetry classes in the even and odd weights. Making use of decompositions like (8.2) and of formulas for indices of plethysms for ordinary symmetry classes,[9] we obtained the following expressions for (second-order) indices of plethysms for Lie superalgebras up to four boxes,

$$I_{\square\square} = NI_\square + 2S_\square + A^2_\square, \tag{8.3}$$

$$I_{\begin{smallmatrix}\square\\\square\end{smallmatrix}} = NI_\square - 2S_\square + A^2_\square, \tag{8.4}$$

$$I_{\square\square\square} = \tfrac{1}{2}(N^2 + N_S + 6)I_\square + 2NS_\square + NA^2_\square + 2A_\square A^S_\square, \tag{8.5}$$

$$I_{\begin{smallmatrix}\square\square\\\square\end{smallmatrix}} = (N^2 - 3)I_\square + 2NA^2_\square, \tag{8.6}$$

$$I_{\begin{smallmatrix}\square\\\square\\\square\end{smallmatrix}} = \tfrac{1}{2}(N^2 - N_S + 6)I_\square - 2NS_\square + NA^2_\square - 2A_\square A^S_\square, \tag{8.7}$$

$$I_{\square\square\square\square} = \tfrac{1}{6}(N^3 + 3NN_S + 20N)I_\square + (N^2 + N_S + 4)S_\square + \tfrac{1}{2}(N^2 + N_S + 4)A^2_\square + (A^S_\square)^2 + 4NA_\square A^S_\square, \tag{8.8}$$

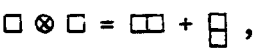
$$I_{\begin{smallmatrix}\square\square\\\square\square\end{smallmatrix}} = \tfrac{1}{2}(N^3 + NN_S)I_\square + (N^2 - N_S - 8)S_\square + \tfrac{1}{2}(3N^2 + N_S)A^2_\square - (A^S_\square)^2 + 2NA_\square A^S_\square, \tag{8.9}$$

$$I_{\begin{smallmatrix}\square\square\\\square\\\square\end{smallmatrix}} = \tfrac{1}{3}(N^3 - 10N)I_\square + 2N_S S_\square + (N^2 - 2)A^2_\square + 2(A^S_\square)^2, \tag{8.10}$$

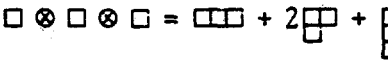
$$I_{\begin{smallmatrix}\square\\\square\\\square\\\square\end{smallmatrix}} = \tfrac{1}{2}(N^3 - NN_S)I_\square - (N^2 + N_S - 8)S_\square + \tfrac{1}{2}(3N^2 - N_S)A^2_\square - (A^S_\square)^2 - 2NA_\square A^S_\square, \tag{8.11}$$

$$I_{\begin{smallmatrix}\square\\\square\\\square\\\square\end{smallmatrix}} = \tfrac{1}{6}(N^3 - 3NN_S + 20N)I_\square - (N^2 - N_S + 4)S_\square + \tfrac{1}{2}(N^2 - N_S + 4)A^2_\square + (A^S_\square)^2 - 4NA_\square A^S_\square. \tag{8.12}$$

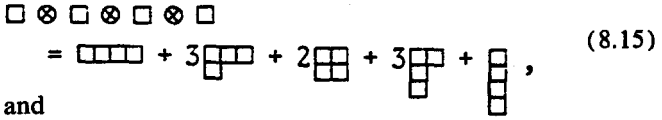
Note that (8.3)–(8.12) can be checked by



(8.13)



(8.14)



(8.15)

and

$$I_{\underbrace{\square\otimes\square\otimes\cdots\otimes\square}_{k\text{ times}}} = kN^{k-1}I_{\square} + k(k-1)N^{k-2}A^2_{\square}. \quad (8.16)$$

For Young tableaux up to four boxes, the superindices are

$$S_{\square\square} = (N_S+2)S_{\square} + (A^S_{\square})^2, \quad (8.17)$$

$$S_{\begin{smallmatrix}\square\\\square\end{smallmatrix}} = (N_S-2)S_{\square} + (A^S_{\square})^2, \quad (8.18)$$

$$S_{\square\square\square} = \tfrac{1}{2}(N_S+2)(N_S+3)S_{\square} + (N_S+2)(A^S_{\square})^2, \quad (8.19)$$

$$S_{\begin{smallmatrix}\square\square\\\square\end{smallmatrix}} = (N_S^2-3)S_{\square} + 2N_S(A^S_{\square})^2, \quad (8.20)$$

$$S_{\begin{smallmatrix}\square\\\square\\\square\end{smallmatrix}} = \tfrac{1}{2}(N_S-2)(N_S-3)S_{\square} + (N_S-2)(A^S_{\square})^2, \quad (8.21)$$

$$S_{\square\square\square\square} = \tfrac{1}{6}(N_S+2)(N_S+3)(N_S+4)S_{\square} + \tfrac{1}{2}(N_S+2)(N_S+3)(A^S_{\square})^2, \quad (8.22)$$

$$S_{\begin{smallmatrix}\square\square\square\\\square\end{smallmatrix}} = \tfrac{1}{2}(N_S+2)(N_S^2+N_S-4)S_{\square} + \tfrac{1}{2}(N_S+2)(3N_S-1)(A^S_{\square})^2, \quad (8.23)$$

$$S_{\begin{smallmatrix}\square\square\\\square\square\end{smallmatrix}} = \tfrac{1}{3}N_S(N_S^2-4)S_{\square} + N_S^2(A^S_{\square})^2, \quad (8.24)$$

$$S_{\begin{smallmatrix}\square\square\\\square\\\square\end{smallmatrix}} = \tfrac{1}{2}(N_S-2)(N_S^2-N_S-4)S_{\square} + \tfrac{1}{2}(N_S-2)(3N_S+1)(A^S_{\square})^2, \quad (8.25)$$

$$S_{\begin{smallmatrix}\square\\\square\\\square\\\square\end{smallmatrix}} = \tfrac{1}{6}(N_S-2)(N_S-3)(N_S-4)S_{\square} + \tfrac{1}{2}(N_S-2)(N_S-3)(A^S_{\square})^2. \quad (8.26)$$

These expressions contain in the rhs only the superdimension, the superindex, and the superanomaly. Again they can be checked by means of (8.13)–(8.15) and

$$S_{\square\otimes\square\otimes\cdots\otimes\square} = kN_S^{k-1}S_{\square} + k(k-1)N_S^{k-2}(A^S_{\square})^2. \quad (8.27)$$

Using a similar method, we obtained expressions for the anomaly and superanomaly for a plethysm:

$$A_{\square\square} = NA_{\square} + A^S_{\square}, \quad (8.28)$$

$$A_{\begin{smallmatrix}\square\\\square\end{smallmatrix}} = NA_{\square} - A^S_{\square}, \quad (8.29)$$

$$A_{\square\square\square} = \tfrac{1}{2}(N^2+N_S+2)A_{\square} + NA^S_{\square}, \quad (8.30)$$

$$A_{\begin{smallmatrix}\square\square\\\square\end{smallmatrix}} = (N^2-2)A_{\square}, \quad (8.31)$$

$$A_{\begin{smallmatrix}\square\\\square\\\square\end{smallmatrix}} = \tfrac{1}{2}(N^2-N_S+2)A_{\square} - NA^S_{\square}, \quad (8.32)$$

$$A_{\square\square\square\square} = \tfrac{1}{6}(N^3+3NN_S+8N)A_{\square} + \tfrac{1}{2}(N^2+N_S+2)A^S_{\square}, \quad (8.33)$$

$$A_{\begin{smallmatrix}\square\square\square\\\square\end{smallmatrix}} = \tfrac{1}{2}(N^3+NN_S)A_{\square} + \tfrac{1}{2}(N^2-N_S-2)A^S_{\square}, \quad (8.34)$$

$$A_{\begin{smallmatrix}\square\square\\\square\square\end{smallmatrix}} = \tfrac{1}{3}(N^3-4N)A_{\square} + N_SA^S_{\square}, \quad (8.35)$$

$$A_{\begin{smallmatrix}\square\square\\\square\\\square\end{smallmatrix}} = \tfrac{1}{2}(N^3-NN_S)A_{\square} - \tfrac{1}{2}(N^2+N_S-2)A^S_{\square}, \quad (8.36)$$

$$A_{\begin{smallmatrix}\square\\\square\\\square\\\square\end{smallmatrix}} = \tfrac{1}{6}(N^3-3NN_S+8N)A_{\square} - \tfrac{1}{2}(N^2-N_S+2)A^S_{\square}; \quad (8.37)$$

$$A^S_{\square\square} = (N_S+1)A^S_{\square}, \quad (8.38)$$

$$A^S_{\begin{smallmatrix}\square\\\square\end{smallmatrix}} = (N_S-1)A^S_{\square}, \quad (8.39)$$

$$A^S_{\square\square\square} = \tfrac{1}{2}(N_S+1)(N_S+2)A^S_{\square}, \quad (8.40)$$

$$A^S_{\begin{smallmatrix}\square\square\\\square\end{smallmatrix}} = (N_S^2-1)A^S_{\square}, \quad (8.41)$$

$$A^S_{\begin{smallmatrix}\square\\\square\\\square\end{smallmatrix}} = \tfrac{1}{2}(N_S-1)(N_S-2)A^S_{\square}, \quad (8.42)$$

$$A^S_{\square\square\square\square} = \tfrac{1}{6}(N_S+1)(N_S+2)(N_S+3)A^S_{\square}, \quad (8.43)$$

$$A^S_{\begin{smallmatrix}\square\square\\\square\square\end{smallmatrix}} = \tfrac{1}{2}(N_S-1)(N_S+1)(N_S+2)A^S_{\square}, \quad (8.44)$$

$$A^S_{\begin{smallmatrix}\square\square\square\\\square\end{smallmatrix}} = \tfrac{1}{3}(N_S-1)N_S(N_S+1)A^S_{\square}, \quad (8.45)$$

$$A^S_{\begin{smallmatrix}\square\square\\\square\\\square\end{smallmatrix}} = \tfrac{1}{2}(N_S+1)(N_S-1)(N_S-2)A^S_{\square}, \quad (8.46)$$

$$A^S_{\begin{smallmatrix}\square\\\square\\\square\\\square\end{smallmatrix}} = \tfrac{1}{6}(N_S-1)(N_S-2)(N_S-3)A^S_{\square}. \quad (8.47)$$

These expressions can be checked making use of (8.13)–(8.15) and

$$A_{\underbrace{\square\otimes\square\otimes\cdots\otimes\square}_{k}} = kN^{k-1}A_{\square},$$

$$A^S_{\underbrace{\square\otimes\square\otimes\cdots\otimes\square}_{k}} = kN_S^{k-1}A^S_{\square}. \quad (8.48)$$

IX. CONCLUSIONS

The purpose of this paper was to define the indices of representations of simple Lie superalgebras and to study their properties. These indices are close analogs of similar objects in the representation theory of simple Lie algebras. It turns out that the definition can proceed in two directions: (i) indices and (ii) superindices. The former are none other than ordinary (Lie algebra) indices typically for semisimple but not simple algebras (or even reductive Lie algebras) and their specific, in general reducible, representations. The relation of the superindex to the index is analogous to that of the supertrace to the trace. Very often it turns out to be zero for irreducible representations. Nevertheless it is a useful quantity as exemplified above, for instance, in computing branching rules; the indices in the reduction must add up to zero.

Our definitions (2.1) and (6.1) follow the original definition[6] of higher indices which, except for the degree 2 index, makes no use of Casimir operators. The index can be defined for every degree (not all properties may exist!) and as such could be related to polynomials in Casimir operators. It may sometimes be advantageous to define the (Lie algebra) indices differently, their existence tied to the existence of Casimir operators.[11,12] We have not pursued this direction here although in our opinion it is a worthwhile and challenging problem.

Applications of the indices are directly proportional to the need to calculate with the representations of simple superalgebras. We have exemplified some obviously useful possibilities like decomposition of tensor products and com-

putation of branching rules. One can also point out physics applications of the (simple Lie algebra) indices in a rather different context.[21] It appears plausible to expect that some version of physics theories in the not too distant future will also involve simple superalgebras.

The concept of indices of representations (like that of the dimension of representation) is more general than has been explicitly explored so far. It hinges on the existence of the weight lattice and thus on the triangular decomposition[22] of the algebra but on little else. As an example let us recall the definition of the dimension and indices in the Kac–Moody situation.[15] While the traditional dimensions and indices would be infinite and hence useless, one has perfectly useful definitions of dimensions and indices (with virtually all the useful properties preserved) as certain power series in one or more variables.

Finally, let us end with a suggestion that a tabulation of the indices for the superalgebras should be a relatively easy task which could be both useful and popular.

ACKNOWLEDGMENT

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Parent potentials for an infinite class of reflectionless kinks

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The sine–Gordon and ϕ-four kinks are known to be reflectionless by virtue of the fact that their small oscillations are governed by the modified Pöschl–Teller potential $U_l(x) = 1 - [(l+1)/l]\mathrm{sech}^2(x/l)$, with $l = 1$ and 2, respectively. An infinite class of parent potentials $V_l(\phi)$ analogous to $V_1 \sim 1 - \cos\phi$ for sine–Gordon kinks and $V_2 \sim (1-\phi^2)^2$ for ϕ-four kinks, which bear reflectionless kinks, are constructed. This is done by requiring the lowest bound-state eigenfunction of $U_l(x)$ to be proportional to the spatial derivative of the kink waveform $\phi_K^{(l)}(x)$, i.e., the translational mode of the kink. The resulting differential equation is solved for $V_l(\phi)$ to find that it can be expressed in terms of the student's t distribution of probability theory. Various properties of the parent potentials and their reflectionless kinks are discussed.

I. INTRODUCTION

The so-called "sine–Gordon" (SG) and "ϕ-four" nonlinear wave equations have found widespread use in recent investigations of solitary-wave (kink) phenomena in both condensed matter physics[1] and particle physics.[2] These two members of the large family[2,3] of nonlinear Klein–Gordon wave equations (possessing particlelike kink solutions) share the remarkable property that they do not reflect incident linearized solutions (e.g., phonons[4]). Although this reflectionless property is not a fundamental requirement for the development of statistical mechanics phenomenologies[4–6] or perturbation theories[7–10] of kink dynamics, it does allow for a simpler treatment than for kinks without this property (e.g., the double-quadratic[5,10] and double-sine–Gordon[6] kinks).

The reflectionless property of the SG and ϕ-four kinks is found by considering the nature of small oscillations about the static kink waveforms. The spatial dependence of these small oscillations (phonons) is governed by an equation of Schrödinger form (see Sec. II below). Remarkably, the "potential" appearing in this pseudo-Schrödinger equation is of the modified Pöschl–Teller[11] type ($\sim -\mathrm{sech}^2 x$) for *both* the SG and ϕ-four cases. For special values[11] of the magnitude of this $\mathrm{sech}^2 x$ potential, incoming "particles" are not reflected but suffer only a phase shift. These special magnitudes for which the potential is reflectionless can be characterized by an integer ($l = 1,2,\ldots,\infty$); it is a curious fact that the appropriate Pöschl–Teller potentials for the SG and ϕ-four problems have $l = 1$ and 2, respectively.

The SG and ϕ-four equations arise from a nonlinear Klein–Gordon Lagrangian in which the self-coupling term ($\sim\phi^2$) is replaced by a nonlinear potential function $V(\phi)$ [$\sim 1 - \cos\phi$ for SG and $\sim(1-\phi^2)^2$ for ϕ-four; see Sec. II]. We call this potential function the "parent potential" for the kink to distinguish it from the potential function which appears in the pseudo-Schrödinger equation for the small oscillations about the kink. Noting that the parent potentials for SG and ϕ-four lead to reflectionless Pöschl–Teller potentials with $l = 1$ and 2, respectively, the question arises as to whether there might exist other parent potentials in the nonlinear Klein–Gordon family which would lead to kinks having Pöschl–Teller potentials with $l = 3$ or higher. If so, then the SG and ϕ-four kinks would be joined by other reflectionless kinks for which the statistical mechanics[3] and dynamics[7] could be treated with ease, since the eigenstates of the Pöschl–Teller potential are known exactly[11] (see Sec. III).

The search for additional parent potentials of reflectionless kinks is not merely an academic exercise. Since the SG and ϕ-four potentials cannot be expected to describe all physical situations of interest (particularly in condensed matter), it would be very beneficial to have additional model kink-bearing potentials at hand for which the small oscillations are known exactly. In this paper, we show how to *explicitly* construct the parent potentials $V_l(\phi)$ for the *entire* infinite class of reflectionless kinks whose associated small oscillations are governed by the modified Pöschl–Teller potentials with $l = 1,2,\ldots,\infty$. We find that there are two subclasses of parent potentials depending on whether l is odd or even. For l odd, the parent potentials are periodic functions of ϕ and SG is the first number ($l = 1$) of this subclass. For l even, the parent potentials have unbounded double-well character and ϕ-four is the first member ($l = 2$) of this subclass.

The outline of the remainder of the paper is as follows. In Sec. II we review the essential features of nonlinear Klein–Gordon kinks and their associated small oscillations. Special attention is paid to the zero-frequency "translation mode"[2–10] which must be present in the spectrum of small oscillations as a consequence of translational invariance. We then specialize to the SG and ϕ-four examples of parent potentials of kinks whose small oscillations are governed by the modified Pöschl–Teller (PT) potential with $l = 1$ and 2, respectively. In Sec. III we collect some of the properties of the reflectionless ($l = 1,2,3,\ldots$) PT eigenstates and give general phase-shift formulas for the continuum states (phonons). In Sec. IV we then construct the parent potentials $V_l(\phi)$ for all $l \geqslant 1$ by requiring the lowest bound-state eigenfunction of the PT potential to be proportional to the spatial derivative of the kink waveform $\phi_K(x)$, i.e., the translation mode of the kink. Although this identification has been noted earlier by Christ and Lee,[12] we actually carry out the explicit construc-

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tion of $V_l(\phi)$ by solving the resulting differential equation for $V_l(\phi)$. We find that the parent potential can be expressed in terms of the student's t distribution of probability theory. Plots of $V_l(\phi)$ are presented for l values up to six. The analytic properties of $V_l(\phi)$ near its degenerate minima are discussed. Finally, in Sec. V we summarize our results and discuss various uses of these higher-order parent potentials.

II. NONLINEAR KLEIN–GORDON KINKS AND THEIR SMALL OSCILLATIONS

In this section we briefly review the derivation of single-kink solutions to the equations of motion of the nonlinear Klein–Gordon variety (e.g., SG and ϕ-four) and the equation of motion for small oscillations about the kinks. We then specialize to the SG and ϕ-four cases as the two well-known examples of reflectionless kinks which have the modified Pöschl–Teller (PT) potential for their small oscillations.

The general nonlinear Klein–Gordon Lagrangian we consider has the dimensionless form

$$L=\int dx\left\{\frac{1}{2}\phi_t^2-\frac{1}{2}\phi_x^2-V(\phi)\right\}, \tag{2.1}$$

where x and t are dimensionless space and time variables, respectively. The nonlinear parent potential $V(\phi)$ is assumed to have at least two degenerate absolute minima, at say ϕ_1 and ϕ_2, such that $V(\phi_1)=V(\phi_2)=0$. In addition, we assume that $V(\phi)$ is scaled in such a way that it has unit positive curvature at its degenerate minima. The nonlinear wave equation satisfied by $\phi(x,t)$ is

$$\phi_{tt}-\phi_{xx}+V'(\phi)=0, \tag{2.2}$$

where the prime on $V(\phi)$ denotes a derivative with respect to ϕ. Static single-kink solutions $\phi_K(x)$ of Eq. (2.2) may be obtained by direct integration with the boundary conditions

$$\left.\frac{d\phi_K(x)}{dx}\right|_{x=\pm\infty}=0 \tag{2.3a}$$

and

$$\phi_K(x=-\infty)=\phi_1,\quad \phi_K(x=+\infty)=\phi_2 \tag{2.3b}$$

for kinks and Eq. (2.3b) with $\phi_1\leftrightarrow\phi_2$ for antikinks (this is the standard convention if $\phi_1<\phi_2$). The kink (+) and antikink (−) solutions are given by

$$x=\pm\frac{1}{\sqrt{2}}\int_{\phi_K(0)}^{\phi_K(x)}\frac{d\phi}{\sqrt{V(\phi)}}. \tag{2.4}$$

Moving kink solutions can be obtained by a Lorentz boost. We shall henceforth be concerned only with the static kink (+) solution since it is not necessary to consider moving kinks in order to derive the general parent potentials of interest (Sec. IV).

The equation governing small oscillations about the static kink waveform is obtained by substituting

$$\phi(x,t)=\phi_K(x)+\psi(x,t) \tag{2.5}$$

into Eq. (2.2) and linearizing in ψ:

$$\psi_{tt}-\psi_{xx}+V''(\phi_K(x))\psi=0. \tag{2.6}$$

Here $V''(\phi_K(x))$ denotes the second derivative of $V(\phi)$ with respect to ϕ evaluated for $\phi=\phi_K(x)$. Writing ψ as

$$\psi(x,t)=f(x)e^{-i\omega t} \tag{2.7}$$

leads to the following eigenvalue equation:

$$-f_{xx}+V''(\phi_K(x))f=\omega^2 f. \tag{2.8}$$

Due to the localized nature of the kink waveform $\phi_K(x)$, the function $V''(\phi_K(x))$ varies mainly in the region near the kink center (assumed to be at $x=0$) and approaches unity (due to our assumption of unit curvature) far away from the kink center,

$$V''(\phi_K(x))\underset{|x|\to\infty}{\to}1. \tag{2.9}$$

Moreover, the function $V''(\phi_K(x))$ has a minimum at $x=0$ such that

$$V''(\phi_K(x))<0. \tag{2.10}$$

From these properties, we see that there exists a close analogy between Eq. (2.8) and the Schrödinger equation for a particle moving in a one-dimensional "potential well," $V''(\phi_K(x))$. The "bound state(s)" and "continuum" states for this potential are of *fundamental* importance for statistical mechanics phenomenologies,[4] perturbation theories of kink dynamics,[7] and quantization procedures for kink states.[2,12–17]

Since the Lagrangian (2.1) possesses translation invariance, the spectrum of small oscillations about a single kink must contain a zero-frequency ($\omega=0$) translation mode (Goldstone mode) that restores the translation invariance broken by the introduction of a kink at $x=0$. This means that Eq. (2.8) must *always* possess a "bound" state solution with $\omega^2=\omega_{b,1}^2=0$ (and perhaps other bound states with $0<\omega^2<1$) and the corresponding bound state wave function $f_{b,1}(x)$ will be proportional to the spatial derivative of $\phi_K(x)$,

$$f_{b,1}(x)\propto\frac{d\phi_K(x)}{dx}, \tag{2.11}$$

as can be shown easily by differentiating Eq. (2.2) with respect to x and setting $\phi=\phi_K(x)$.

In addition to the translation mode at $\omega^2=0$, there may exist additional bound state solutions of Eq. (2.8) with nonzero frequencies (between 0 and 1). The solutions correspond to "internal" oscillation modes in which the kink waveform undergoes a harmonically varying shape change localized about the kink center. We denote the bound-state eigenfrequencies by $\omega_{b,1}=0, \omega_{b,2},\ldots,\omega_{b,N_b}$, where N_b is the total number of bound states. The lowest of these is $\omega_{b,1}=0$ (the translation mode) since all other $\omega_{b,n}^2$ must be nonnegative in order for the kink to be stable against small oscillations.

In addition to the bound-state solutions of Eq. (2.8), there exist continuum states (extended modes) which we label by a wave vector k. These states have eigenvalues ω_k^2 given by

$$\omega_k^2=1+k^2, \tag{2.12}$$

which is precisely the dispersion relation for small oscillations (phonons) in the *absence* of kinks. Equation (2.12) follows from the fact that far away from the kink the poten-

tial $V''(\phi_K(x))$ approaches unity [Eq. (2.9)]. Although the precise form of the continuum eigenfunction $f_k(x)$ can be quite complicated in the region of the kink, it has the following simple asymptotic form for the reflectionless potentials $V''(\phi_K(x))$ which we consider in this paper:

$$f_k(x) \underset{x\to\pm\infty}{\to} A_k \exp i[kx \pm \tfrac{1}{2}\Delta(k)], \tag{2.13}$$

where $\Delta(k)$ is a phase-shift function which depends on the potential at hand. This phase-shift function is an extremely important quantity since it contains all the information concerning kink–phonon interactions that is needed to renormalize the kink energy due to thermal[4] or quantum[14] fluctuations (or both[17]).

Now we consider the SG and ϕ-four cases in particular. The parent potentials are

$$V_1(\phi) = 1 - \cos\phi \quad \text{(SG)}, \tag{2.14a}$$

$$V_2(\phi) = \tfrac{1}{8}(\phi^2 - 1)^2 \quad (\phi\text{-four}), \tag{2.14b}$$

where the meaning of the subscripts 1 and 2 will become clear in a moment. The static single-kink solutions are

$$\phi_K(x) = 4\tan^{-1} e^x \quad \text{(SG)}, \tag{2.15a}$$

$$\phi_K(x) = \tanh(x/2) \quad (\phi\text{-four}). \tag{2.15b}$$

For future reference we give the dimensionless energies of the static kinks obtained from the general relation,[4]

$$E_K = 2\int_{-\infty}^{+\infty} dx\, V(\phi_K(x)) = \sqrt{2}\int_{\phi_1}^{\phi_2} d\phi\sqrt{V(\phi)}\,. \tag{2.16}$$

These are

$$E_K = 8 \quad \text{(SG)}, \tag{2.17a}$$

$$E_K = \tfrac{2}{3} \quad (\phi\text{-four}). \tag{2.17b}$$

From Eqs. (2.14) and (2.15) it is straightforward to derive the potential function $V''(\phi_K(x))$ which appears in Eq. (2.8). We find

$$V_1''(\phi_K(x)) = 1 - 2\,\mathrm{sech}^2 x \quad \text{(SG)}, \tag{2.18a}$$

$$V_2''(\phi_K(x)) = 1 - \tfrac{3}{2}\,\mathrm{sech}^2(x/2) \quad (\phi\text{-four}). \tag{2.18b}$$

These two potentials are special cases ($l = 1$ and 2, respectively) of the modified Pöschl–Teller (PT) potential,[11]

$$U_l(x) = 1 - [(l+1)/l]\,\mathrm{sech}^2(x/l), \tag{2.19}$$

for which the exact eigenstates are known analytically.[11] The SG case has exactly one bound state (the translation mode),

$$f_{b,1}(x) = (1/\sqrt{2})\,\mathrm{sech}\, x, \quad \omega_{b,1}^2 = 0, \tag{2.20}$$

and the continuum states

$$f_k(x) = [2\pi(1+k^2)]^{-1/2} e^{ikx}(k + i\tanh x). \tag{2.21}$$

The ϕ-four case has *two* bound states,

$$f_{b,1}(x) = \tfrac{1}{2}\sqrt{\tfrac{3}{2}}\,\mathrm{sech}^2(x/2), \quad \omega_{b,1}^2 = 0, \tag{2.22a}$$

$$f_{b,2}(x) = \tfrac{1}{2}\sqrt{3}\,\mathrm{sech}(x/2)\tanh(x/2), \quad \omega_{b,2}^2 = \tfrac{3}{4}, \tag{2.22b}$$

and the continuum states

$$f_k(x) = [8\pi(1+k^2)(1+4k^2)]^{-1/2} e^{ikx} \times (3\tanh^2(x/2) - 6ik\tanh(x/2) - [1+4k^2]). \tag{2.23}$$

These states satisfy the orthonormality conditions

$$\int_{-\infty}^{+\infty} dx\, f_{b,n}(x) f_{b,m}(x) = \delta_{n,m}\,, \tag{2.24a}$$

$$\int_{-\infty}^{+\infty} dx\, f_k^*(x) f_{k'}(x) = \delta(k-k'), \tag{2.24b}$$

$$\int_{-\infty}^{+\infty} dx\, f_k(x) f_{b,n}(x) = 0, \tag{2.24c}$$

and the completeness relation,

$$\sum_{n=1}^{N_b} f_{b,n}(x) f_{b,n}(x') + \int_{-\infty}^{+\infty} dk\, f_k^*(x) f_k(x') = \delta(x-x'). \tag{2.25}$$

From Eqs. (2.21) and (2.23) we find the phase shift function defined in Eq. (2.13):

$$\Delta_1(k) = \pi(k/|k|) - 2\tan^{-1} k \quad \text{(SG)}, \tag{2.26a}$$

$$\Delta_2(k) = 2\pi(k/|k|) - 2\tan^{-1} k - 2\tan^{-1} 2k \quad (\phi\text{-four}). \tag{2.26b}$$

III. EIGENSTATES OF THE REFLECTIONLESS MODIFIED PÖSCHL–TELLER POTENTIAL

In this section we collect some of the useful properties of the eigenstates of the modified PT potential (2.19) for arbitrary positive values of the integer index l. In the next section we shall construct the parent potentials $V_l(\phi)$ for which the small oscillations about the kink solutions satisfy Eq. (2.8) with the PT potential,

$$V_l''(\phi_K(x)) = 1 - [(l+1)/l]\,\mathrm{sech}^2(x/l), \tag{3.1}$$

namely,

$$-\frac{d^2 f^{(l)}}{dx^2} + \left[1 - \frac{l+1}{l}\,\mathrm{sech}^2\frac{x}{l}\right] f^{(l)} = \omega^2 f^{(l)}\,. \tag{3.2}$$

Using the substitution $\eta = \tanh(x/l)$, this equation becomes the associated Legendre equation[18]

$$(1-\eta^2)\frac{d^2 f^{(l)}}{d\eta^2} - 2\eta\frac{df^{(l)}}{d\eta} + \left[l(l+1) - \frac{l^2(1-\omega^2)}{1-\eta^2}\right] f^{(l)} = 0\,. \tag{3.3}$$

The normalized bound state solutions are

$$f_{b,n}^{(l)}(x) = \left\{\frac{(l-n+1)(n-1)!}{l(2l-n+1)!}\right\}^{1/2} P_l^{l-n+1}\left(\tanh\frac{x}{l}\right) \quad (n = 1,2,\ldots,l)\,, \tag{3.4}$$

with eigenvalues

$$\omega_{b,n}^2 = 1 - [1 - [(n-1)/l]]^2\,. \tag{3.5}$$

The function $P_l^{l-n+1}(\tanh(x/l))$ is the associated Legendre polynomial.[18] The continuum states are

$$f_k^{(l)}(x) = A_k^{(l)} P_l^{ik}(\tanh(x/l)), \tag{3.6}$$

where $A_k^{(l)}$ is a normalization constant which we will not need for our purposes. Using the expression of $P_\mu^\nu(z)$ in

terms of the hypergeometric function,[19] we can write

$$f_k^{(l)}(x) = \frac{A_k^{(l)}}{\Gamma(1-ilk)} \times e^{ikx} F(-l,\ l+1;\ 1-ilk;\ \tfrac{1}{2}[1-\tanh(x/l)]). \tag{3.7}$$

This hypergeometric function F is simply a polynomial of degree l in the variable, $1-\tanh x/l$. From its asymptotic behavior[20] we can calculate the phase shift function $\Delta_l(k)$

$$\Delta_l(k) = l\pi\frac{k}{|k|} - 2\sum_{n=1}^{l}\tan^{-1}\left(\frac{lk}{n}\right). \tag{3.8}$$

The only state which we shall need in order to construct these parent potentials is the ground state (translation mode),

$$f_{b,1}^{(l)}(x) = [(2l-1)!!/2^l l!]^{1/2}\operatorname{sech}^l(x/l). \tag{3.9}$$

IV. CONSTRUCTION OF THE PARENT POTENTIALS

We seek the parent potentials $V_l(\phi)$ whose daughter kinks $\phi_K(x)$ are reflectionless by virtue of the potentials they present to small oscillations,

$$V_l''(\phi_K(x)) \equiv 1 - [(l+1)/l]\operatorname{sech}^2(x/l). \tag{4.1}$$

From Eq. (2.11) we know that the translation mode $f_{b,1}^{(l)}(x)$ [Eq. (3.9)] is proportional to $d\phi_K(x)/dx$. Let the proportionality constant be denoted by α_l; it will be chosen later in a convenient manner. Thus we have

$$f_{b,1}^{(l)}(x) = \alpha_l\frac{d\phi_K(x)}{dx}. \tag{4.2}$$

From Eq. (2.4), $d\phi_K/dx$ can be expressed in terms of V_l itself,

$$\frac{d\phi_K}{dx} = [2\,V_l(\phi_K(x))]^{1/2}. \tag{4.3}$$

Combining Eqs. (3.9), (4.2), and (4.3), we have

$$\operatorname{sech}^l(x/l) = \alpha_l[2^l l!/(2l-1)!!]^{1/2}[2\,V_l(\phi_K(x))]^{1/2}. \tag{4.4}$$

Substitution of Eq. (4.4) into Eq. (4.1) then yields

$$V_l''(\phi_K(x)) = 1 - [(l+1)/l]\,[V_l(\phi_K(x))/V_l^0]^{1/l}, \tag{4.5}$$

where

$$V_l^0 \equiv (1/\alpha_l^2)[(2l-1)!!/2^{l+1}l!] \tag{4.6}$$

is the height of the barrier between adjacent minima (at ϕ_1 and ϕ_2) in the parent potential, as can be seen by setting $x=0$ in Eq. (4.4).

Equation (4.5) provides a differential equation for $V_l(\phi)$ for all values of ϕ between ϕ_1 and ϕ_2 [the range swept by the kink $\phi_K(x)$]. Thus

$$\frac{d^2V_l(\phi)}{d\phi^2} = 1 - \frac{l+1}{l}\left[\frac{V_l(\phi)}{V_l^0}\right]^{1/l} \quad (\phi_1<\phi<\phi_2). \tag{4.7}$$

We remark that the positive real branch of the lth root of $V_l(\phi)/V_l^0$ must be chosen in Eq. (4.7), to be consistent with Eq. (4.4) for $\phi_1<\phi<\phi_2$. Although Eq. (4.7) was derived assuming ϕ is in the kink range, we may obtain $V_l(\phi)$ for ϕ outside this range by an appropriate analytic continuation. It is convenient to proceed separately for the cases l odd and l even.

(i) l odd: All of the parent potentials in this class are periodic functions of ϕ with period $\phi_2-\phi_1$; they have the same topology as SG ($l=1$) which is the first member of the class. It is therefore convenient for l odd to choose $\phi_1=0$ and $\phi_2=2\pi$ so that all of these potentials have period 2π. This choice fixes the barrier height V_l^0, which in turn determines the constant α_l via Eq. (4.6). Furthermore, we see from Eq. (4.7) that $V_l(\phi)$ can be made symmetric in ϕ,

$$V_l(-\phi) = V_l(\phi). \tag{4.8}$$

Combining this symmetry with the periodicity property, we see that $V_l(\phi)$ is also symmetric about π. Thus we need only integrate Eq. (4.7) in the range $0<\phi<\pi$. The first integral is easily obtained,

$$\frac{dV_l(\phi)}{d\phi} = [2V_l(\phi)]^{1/2}\left\{1-\left[\frac{V_l(\phi)}{V_l^0}\right]^{1/l}\right\}^{1/2}. \tag{4.9}$$

Integrating once more, we have

$$\phi = \frac{1}{\sqrt{2}}\int_0^{V_l(\phi)}\frac{dV}{\sqrt{V}}\left\{1-\left[\frac{V}{V_l^0}\right]^{1/l}\right\}^{-1/2}. \tag{4.10}$$

This equation gives an implicit solution for $V_l(\phi)$ for $0<\phi<\pi$, and can be reexpressed in several equivalent forms. Defining

$$\xi_l = [V_l(\phi)/V_l^0]^{1/2l}, \tag{4.11}$$

we can write

$$\phi = l(2V_l^0)^{1/2}\int_0^{\sin^{-1}\xi_l} d\theta\,\sin^{l-1}\theta \tag{4.12}$$

$$= l(2V_l^0)^{1/2}\int_0^{\xi_l} dy\,y^{l-1}(1-y^2)^{-1/2} \tag{4.13}$$

$$= l\left(\frac{V_l^0}{2}\right)^{1/2}B\left(\frac{l}{2},\frac{1}{2}\right)I_{\xi_l^2}\left(\frac{l}{2},\frac{1}{2}\right), \tag{4.14}$$

where $I_x(a,b)$ is the normalized incomplete beta function[21] and $B(a,b)$ is the beta function.[22] Here $B(a,b)$ may be expressed[22] in terms of gamma functions by

$$B(a,b) = \Gamma(a)\Gamma(b)/\Gamma(a+b). \tag{4.15}$$

The function $I_x(a,b)$ lies in the unit interval: $I_0(a,b)=0$, $I_1(a,b)=1$. The barrier height V_l^0 is now determined by noting that $\phi=\pi$ is the midpoint of the barrier and $\xi_l=1$ at this point. Thus from Eq. (4.14) we have

$$V_l^0 = 2\pi^2/l^2B^2(l/2,\tfrac{1}{2}) \quad (l \text{ odd}). \tag{4.16}$$

Equation (4.14) then becomes

$$\phi = \pi I_{\xi_l^2}(l/2,\tfrac{1}{2}). \tag{4.17}$$

Because of the particular values of the indices of the incomplete beta function appearing in Eq. (4.17), we can relate $I_{\xi_l^2}(l/2,\frac{1}{2})$ to the so-called "student's t distribution," [21] $A(t\,|l)$ which arises in the theory of probability distribution functions.[21] Namely,

$$I_{\xi_l^2}(l/2,\tfrac{1}{2}) = 1 - A(t\,|l), \tag{4.18}$$

where

$$t \equiv \sqrt{l}\left[(\sqrt{1-\xi_l^2})/\xi_l\right]. \tag{4.19}$$

Thus

$$1-\phi/\pi = A(t\,|l) \quad (0\leqslant\phi\leqslant\pi) \quad (l \text{ odd}). \tag{4.20}$$

If we denote the inverse of the student's t distribution function by $A_l^{-1}(x)$, then

$$t = A_l^{-1}(1-\phi/\pi). \tag{4.21}$$

From Eq. (4.19), we have

$$\xi_l^2 = l/(l+t^2). \tag{4.22}$$

Hence, using Eqs. (4.11), (4.21), and (4.22), we finally obtain a formal expression for the normalized parent potential $\tilde{V}_l(\phi) \equiv V_l(\phi)/V_l^0$,

$$\tilde{V}_l(\phi) = \{l/(l+[A_l^{-1}(1-\phi/\pi)]^2)\}^l \quad (l \text{ odd};\ 0\leqslant\phi\leqslant\pi). \tag{4.23}$$

For ϕ outside this range, $\tilde{V}_l(\phi)$ is continued from Eq. (4.23) using

$$\tilde{V}_l(2\pi-\phi) \equiv \tilde{V}_l(\phi) = \tilde{V}_l(\phi+2\pi n), \tag{4.24}$$

where n is any integer.

Although Eqs. (4.23) and (4.24) represent the formal solution to the problem of finding the periodic (l odd) parent potentials, it is not convenient to use Eq. (4.23) directly if one wishes, for example, to obtain a plot of $\tilde{V}_l(\phi)$ vs ϕ. Instead, it is much easier to obtain ϕ in terms of $\tilde{V}_l$ by making use of Eq. (4.20) and a finite series expansion[21,23] of the student's t distribution,

$$A(t\,|l) = \frac{2}{\pi}\left\{\theta + \sin\theta \sum_{n=1}^{(l-1)/2} \frac{(2n-2)!!}{(2n-1)!!}\cos^{2n-1}\theta\right\}, \tag{4.25}$$

where

$$\theta \equiv \tan^{-1}(t/\sqrt{l}). \tag{4.26}$$

Using Eq. (4.22) we can reexpress θ as

$$\theta = \cos^{-1}\xi_l \tag{4.27}$$

and from Eqs. (4.20), (4.11), (4.25), and (4.26) we then have

$$\frac{\pi-\phi}{2} = \cos^{-1}\tilde{V}_l^{1/2l} + \{1-\tilde{V}_l^{1/l}\}^{1/2}\sum_{n=1}^{(l-1)/2}\frac{(2n-2)!!}{(2n-1)!!}\tilde{V}_l^{(n-1/2)/l}. \tag{4.28}$$

Equation (4.28) provides a simple, explicit expression for ϕ as a function of $\tilde{V}_l$ which may be plotted in the range $0\leqslant\phi\leqslant\pi$, $0\leqslant\tilde{V}_l\leqslant 1$. The curve thus obtained can then be inverted and extended to include several periods of $\tilde{V}_l(\phi)$ using Eq. (4.24) if desired. In Fig. 1, we show the results of this procedure for $l=3$ and 5, in addition to a plot of $\tilde{V}_1(\phi) = \frac{1}{2}(1-\cos\phi)$, which is the sine–Gordon potential. Note the tendency for the barrier between adjacent minima to become more plateaulike as l is increased. Indeed, this behavior becomes extreme in the limit as $l\to\infty$. This can be seen from

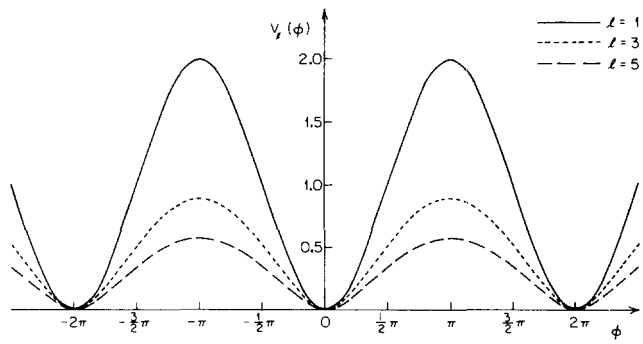

FIG. 1. The first three periodic parent potentials (l odd).

the limit of the student's t distribution,

$$\lim_{l\to\infty} A(t\,|l) \equiv A(t) = \frac{1}{\sqrt{2\pi}}\int_{-t}^{t} e^{-x^2/2}\,dx = \operatorname{erf}(\sqrt{2}\,t), \tag{4.29}$$

where $\operatorname{erf}(\sqrt{2}\,t)$ is the error function.[24] Thus using Eqs. (4.11), (4.19), and (4.20), we have in the limit $l\to\infty$

$$\phi/\pi = \lim_{l\to\infty}\operatorname{erfc}\left[\sqrt{2l}\{(1-\tilde{V}_l^{1/l})/\tilde{V}_l^{1/l}\}^{1/2}\right], \tag{4.30}$$

where $\operatorname{erfc} z = 1 - \operatorname{erf} z$ is the complimentary error function.[24] Since this function becomes very sharply peaked as a function of $[(1-\tilde{V}_l^{1/l})/\tilde{V}_l^{1/l}]^{1/2}$ when l becomes large, we see that $\tilde{V}_l^{1/l}$ (and hence $\tilde{V}_l$) must remain very close to unity as ϕ is decreased from π until ϕ nears zero at which point $\tilde{V}_l$ must drop sharply to zero. We note, however, that the barrier height V_l^0 tends to zero in the large l limit as

$$V_l^0 \underset{l\to\infty}{\to} \pi/l \tag{4.31}$$

as can be shown from Eqs. (4.15) and (4.16) and the use of Sterling's asymptotic formula[22] for the gamma function.

(ii) l even: All of the parent potentials in this class have the same topology as the ϕ-four potential ($l=2$), namely a double-well structure. It is therefore convenient for l even to

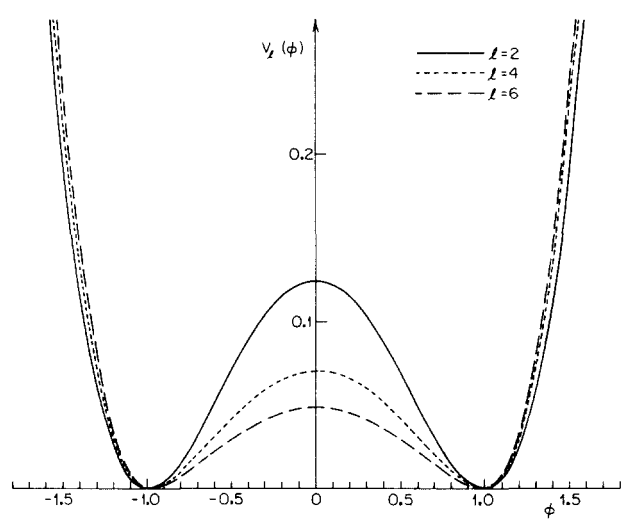

FIG. 2. The first three double-well parent potentials (l even). For $\phi\approx 2.1$, the curves cross so that for fixed $\phi_0 \gtrsim 2.1$, $V_2(\phi_0) > V_4(\phi_0) > V_6(\phi_0)$.

choose $\phi_1 = -1$ and $\phi_2 = +1$ so that all of these potentials have their two degenerate well-minima located at $\phi = \pm 1$. With this choice the potential is symmetric about $\phi = 0$, where the barrier has its maximum V_l^0. Thus to first obtain $V_l(\phi)$ in the kink range, $-1 \leqslant \phi \leqslant +1$, we need only integrate Eq. (4.7) in the range $0 \leqslant \phi \leqslant 1$. The slope of $V_l(\phi)$ is negative in this range, so that the first integral of Eq. (4.7) is

$$\frac{dV_l(\phi)}{d\phi} = -[2V_l(\phi)]^{1/2}\left\{1 - \left[\frac{V_l(\phi)}{V_l^0}\right]^{1/l}\right\}^{1/2}. \quad (4.32)$$

Integrating once more we have

$$\phi = -\frac{1}{\sqrt{2}}\int_{V_l^0}^{V_l(\phi)} \frac{dV}{\sqrt{V}}\left\{1 - \left(\frac{V}{V_l^0}\right)^{1/l}\right\}^{-1/2} \quad (4.33)$$

$$= -l(2V_l^0)^{1/2}\int_1^{\xi_l} dy\, y^{l-1}(1-y^2)^{-1/2}$$

$$= l(2V_l^0)^{1/2}\left[\int_0^1 dy\, y^{l-1}(1-y^2)^{-1/2} - \int_0^{\xi_l} dy\, y^{l-1}(1-y^2)^{-1/2}\right] \quad (4.34)$$

$$= l\left[\frac{V_l^0}{2}\right]^{1/2} B\left(\frac{l}{2},\frac{1}{2}\right)\left[1 - I_{\xi_l^2}\left(\frac{l}{2},\frac{1}{2}\right)\right]. \quad (4.35)$$

Noting that when $\phi = 1$, ξ_l^2 must equal zero [Eq. (4.11)], we then obtain an expression for the barrier height when l is even,

$$V_l^0 = 2/l^2 B^2(l/2,\tfrac{1}{2}) \quad (l \text{ even}). \quad (4.36)$$

Equation (4.35) then becomes

$$1 - \phi = I_{\xi_l^2}(l/2,\tfrac{1}{2}) \quad (0 \leqslant \phi \leqslant 1), \quad (4.37)$$

or, using the student's t distribution,

$$\phi = A(t\,|l). \quad (4.38)$$

This may be formally inverted as for the odd l case to give the normalized parent potential

$$\tilde{V}_l(\phi) = \{l/(l + [A_l^{-1}(\phi)]^2)\}^l \quad (l \text{ even};\ 0 \leqslant \phi \leqslant 1). \quad (4.39)$$

Equation (4.38) can be made more explicit by using the series expansion for $A(t\,|l)$ when l is even[21]:

$$A(t\,|l) = \sin\theta\left\{1 + \sum_{n=1}^{l/2-1}\frac{(2n-1)!!}{(2n)!!}\cos^{2n}\theta\right\}, \quad (4.40)$$

where θ is given in terms of t by Eq. (4.26) and in terms of ξ_l by Eq. (4.27). Thus Eq. (4.38) can be rewritten as

$$\phi = \{1 - \tilde{V}_l^{1/l}\}^{1/2}\left[1 + \sum_{n=1}^{l/2-1}\frac{(2n-1)!!}{(2n)!!}\tilde{V}_l^{n/l}\right] \quad (l \text{ even};\ 0 \leqslant \phi \leqslant 1), \quad (4.41)$$

where we have used Eq. (4.11).

To obtain results for $|\phi| > 1$ we return to Eq. (4.32), where we note that if $V_l(\phi) \to \infty$ as $|\phi| \to \infty$ for each l, the slope becomes imaginary when $\tilde{V}_l > 1$. Choosing the negative real root of $(\tilde{V}_l)^{1/l}$ avoids this problem and exactly reproduces the ϕ-four solution (for $l = 2$). Since $V(\phi) = V(-\phi)$ we restrict our attention to $\phi > 1$ where the slope $dV_l/d\phi > 0$ and write

$$\frac{dV_l}{d\phi} = \sqrt{2V_l(\phi)}\left[1 + \left(\frac{V_l(\phi)}{V_l^0}\right)^{1/l}\right]^{1/2}. \quad (4.42)$$

Hence

$$\phi - 1 = \frac{1}{\sqrt{2}}\int_0^{V_l(\phi)}\frac{dV}{\sqrt{V}}\left[1 + \left(\frac{V}{V_l^0}\right)^{1/l}\right]^{-1/2} \quad (4.43)$$

$$= l\sqrt{2V_l^0}\int_0^{\sinh^{-1}\xi_l}(\sinh x)^{l-1}\,dx \quad (4.44)$$

$$= l\sqrt{2V_l^0}(-1)^{(l-2)/2}\sum_{n=0}^{(l-2)/2}(-1)^n\binom{\frac{l-2}{2}}{n} \times \frac{1}{2n+1}[(\xi_l^2+1)^{(2n+1)/2} - 1]. \quad (4.45)$$

Therefore

$$\phi = 1 + l\sqrt{2V_l^0}(-1)^{(l-2)/2} \times \sum_{n=0}^{(l-2)/2}(-1)^n\binom{(l-2)/2}{n} \times \frac{1}{2n+1}\left\{\left[\left(\frac{V_l}{V_l^0}\right)^{1/l} + 1\right]^{(2n+1)/2} - 1\right\} \quad (l \text{ even};\ \phi \geqslant 1). \quad (4.46)$$

Equations (4.41) and (4.46) can be used to obtain ϕ vs $\tilde{V}_l(\phi)$ plots for all $\phi \geqslant 0$, whereupon the plots can be inverted to give $\tilde{V}_l(\phi)$. For $\phi < 0$, we use the symmetry of $\tilde{V}_l$: $\tilde{V}_l(-\phi) = \tilde{V}_l(\phi)$. In Fig. 2 we show the results of this procedure for $l = 4$ and 6, as well as the ϕ-four parent potential for comparison.

Apart from the ϕ-four case ($l = 2$), the only other case for which Eqs. (4.41) and (4.46) can be inverted analytically is $l = 4$. In this case, they become third degree polynomials in $\xi_4^2 = \tilde{V}_4^{1/4}$ whose roots can be found in closed form[25]:

$$\tilde{V}_4(\phi) = \begin{cases} [2\cos(\frac{1}{3}\sin^{-1}\phi) - 1]^4, & 0 \leqslant |\phi| \leqslant 1, \\ [\cos(\frac{1}{3}\sin^{-1}(\phi-2)) + \sqrt{3}\sin(\frac{1}{3}\sin^{-1}(\phi-2)) + 1]^4, & 1 \leqslant |\phi| \leqslant 3, \\ [2\cosh(\frac{1}{3}\cosh^{-1}(\phi-2)) + 1]^4, & |\phi| \geqslant 3. \end{cases} \quad (4.47)$$

TABLE I. Barrier heights and kink rest energies for the first six parent potentials.

l	V_l^0	$E_K^{(l)}$
1	2	8
2	$\frac{1}{8}$	$\frac{2}{3}$
3	$\frac{8}{9}$	$\frac{256}{45}$
4	$\frac{9}{128}$	$\frac{18}{35}$
5	$\frac{128}{225}$	$\frac{65\,536}{14\,175}$
6	$\frac{25}{512}$	$\frac{100}{231}$

From Eqs. (2.16) and (4.9), we can obtain a simple expression for the kink rest energies, $E_K^{(l)}$, for odd l,

$$E_K^{(l)} = \sqrt{2}\int_{\phi_1}^{\phi_2} d\phi\,[V_l(\phi)]^{1/2}$$
$$= 2\sqrt{2}\int_0^{V_l^0} dV\left(\frac{dV}{d\phi}\right)^{-1}\sqrt{V}$$
$$= 2lV_l^0\int_0^1 dz\, z^{l-1}(1-z)^{-1/2}$$

or

$$E_K^{(l)} = 2lV_l^0 B(l,\tfrac{1}{2}). \tag{4.48}$$

This result also holds for l even. Using Eqs. (4.15), (4.16), and (4.36), we have calculated the parent potential barrier heights V_l^0 and kink rest energies for the first several values of l and for convenience listed these in Table I.

The coefficients α_l in Eq. (4.2) can be shown, using Eqs. (4.6) and (4.48), to be simply related to the kink rest energies via

$$\alpha_l = [E_K^{(l)}]^{-1/2}. \tag{4.49}$$

The actual static kink waveforms can be obtained from Eqs. (4.2), (4.6), and (3.9) in a straightforward manner,

$$\frac{d\phi_K^{(l)}(x)}{dx} = \alpha_l^{-1} f_{b,1}^{(l)}(x)$$
$$= (2V_l^0)^{1/2}\,\mathrm{sech}^l(x/l). \tag{4.50}$$

Thus

$$\phi_K^{(l)}(x) = l(2V_l^0)^{1/2}\int^{x/l} dy\,\mathrm{sech}^l y, \tag{4.51}$$

where the lower limit on the integration is unnecessary since its contribution has been cancelled by ϕ_1 on the left-hand side. The indefinite integral of $\mathrm{sech}^l y$ can be found in the tables of Ref. 26. We present explicit forms for l up to 6 in Table II and in Figs. 3 and 4 we plot the waveforms for these six reflectionless kinks.

TABLE II. Static waveforms for the first six reflectionless kinks.

l	$\phi_K^{(l)}(x)$
1	$4\tan^{-1}e^x$
2	$\tanh(x/2)$
3	$4\tan^{-1}e^{x/3} + 2\,\mathrm{sech}(x/3)\tanh(x/3)$
4	$\frac{3}{2}\tanh(x/4)[1-\frac{1}{3}\tanh^2(x/4)]$
5	$4\tan^{-1}e^{x/5} + [\frac{4}{3}\mathrm{sech}^3(x/5) + 2\,\mathrm{sech}(x/5)]\tanh(x/5)$
6	$\frac{15}{8}\tanh(x/6)[1-\frac{2}{3}\tanh^2(x/6)+\frac{1}{5}\tanh^4(x/6)]$

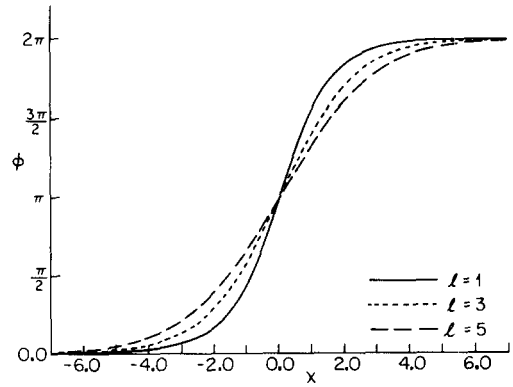

FIG. 3. Static kink waveforms for $l = 1$ (SG), 3, and 5.

The analytic properties of the parent potential $V_l(\phi)$ can be exhibited by considering its successive derivatives near one of its degenerate minima. By construction, the first derivative vanishes at ϕ_1 or ϕ_2, and the second derivative approaches unity at these values. The third derivative can be obtained from Eqs. (4.7) and (4.9) (or 4.32),

$$\frac{d^3V_l(\phi)}{d\phi^3} = \pm\sqrt{2}\,\frac{l+1}{l^2}\,[V_l^0]^{-1/l}[V_l(\phi)]^{1/l-1/2}$$
$$\times\left\{1-\left[\frac{V_l(\phi)}{V_l^0}\right]^{1/l}\right\}^{1/2}. \tag{4.52}$$

As ϕ approaches a potential minimum from small $|\phi|$ values, $V_l(\phi)$ approaches zero, so that

$$\frac{d^3V_l(\phi)}{d\phi^3} \underset{\phi\to\phi_{1,2}}{\to} \pm\sqrt{2}\,\frac{l+1}{l^2}\,[V_l^{(0)}]^{-1/l}[V_l(\phi)]^{1/l-1/2} \tag{4.53}$$

and we see that for $l > 2$, the third (and higher) derivatives are singular at the well minima. (This fact has been noted previously by Christ and Lee[12].) Thus the parent potentials for $l > 2$ do not possess Taylor expansions about their minima. Although the parent potentials and their first two de-

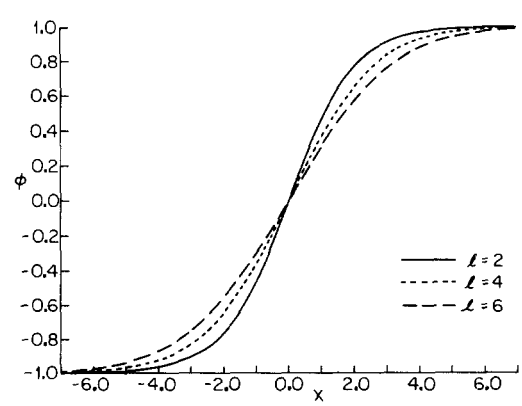

FIG. 4. Static kink waveforms for $l = 2$ (ϕ-four), 4, and 6.

rivatives are continuous, the singularities in their higher derivatives can be expected to cause difficulties in calculations which incorporate these derivatives; for example: high-order perturbation theories of kink response to external forces,[7–10] "anharmonic phonon" contributions to statistical mechanical quantities,[3–6] and quantum renormalization[2,12–17] of kink energies. Nevertheless, if one is interested only in the lowest-order "Gaussian" fluctuations about the kink solutions, the parent potentials we have constructed in this section are well-behaved to this order.

V. SUMMARY AND DISCUSSION

In this paper we have obtained the formal solution [Eqs. (4.23) and (4.29)] to the problem of finding parent potentials for an infinite class of nonlinear Klein–Gordon kinks which are reflectionless by virtue of the fact that they present a modified Pöschl–Teller potential of special magnitude to the small oscillations (e.g., phonons). We found that these parent potentials $V_l(\phi)$ fall into two subclasses: for l odd they are periodic functions of the field ϕ and the sine–Gordon potential is the first member ($l=1$) of this subclass; for l even they have double-well structure, and the ϕ-four potential is the first member ($l=2$) of this subclass.

Although the SG and ϕ-four potentials are the only members of this class which can be expressed as Taylor series in ϕ, the entire class of parent potentials enjoys (by construction) the very attractive feature that the spectra of small oscillations about the kink solutions are known exactly (Sec. III). This knowledge allows a rather complete construction of kink-gas phenomenologies for the low-temperature statistical mechanics[4] of the entire class, and the derivation of generalized susceptibilities[8,10] of the kinks to external perturbations. These topics will be discussed in subsequent papers.

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On the τ-functions of $A_2^{(2)}$

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A general construction of partial differential equations satisfied by the components of τ-functions is given by considering the tensor products of modules. This procedure is applied to the $A_2^{(2)}$-modules $L(\Lambda_0)$ and $L(\Lambda_1)$, leading to the Kaup equation and Sawada–Kotera equation, respectively. Although $L(\Lambda_0)$ and $L(\Lambda_1)$ are of different level, one can consider $L(\Lambda_0)\otimes L(\Lambda_1)$, leading to so-called modified equations. This last construction is new, and leads to a different choice of y, the variable that generates the equations.

I. INTRODUCTION

Some years ago, Date *et al.*[1] and Jimbo and Miwa[2] showed that solutions of many soliton equations can be considered as a group orbit of a highest weight vector v_Λ of $L(\Lambda)$. Here $L(\Lambda)$ is the irreducible affine Lie algebra module with highest weight Λ.

In those papers these representations are found by restricting representations of Clifford algebras to the Lie algebra one is interested in. The purpose of this paper is to show that one can do without these Clifford algebras of "fermions." The derivation of equations (in the spirit of Kac[3]) is by considering tensor modules. In this way one is less restricted in the algebra one wants to consider, and one has more freedom in the representation under consideration. Moreover, one gets a better insight into the τ-functions involved.

This paper is an application and extension of Ref.4; here we only consider $A_2^{(1)}$ and $A_2^{(2)}$.

II. EQUATIONS CORRESPONDING TO A LIE ALGEBRA MODULE

We explain how one can construct partial differential equations corresponding to an affine Lie algebra $\mathbf{g}(A)$ and certain realizations of integrable irreducible representations $L(\Lambda)$ (cf. Ref. 4). We take

$$A=\begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix}$$

or

$$A=\begin{pmatrix} 2 & -1 \\ -4 & 2 \end{pmatrix}$$

and $\Lambda=\Lambda_i$ throughout this paper.

Let $\mathbf{g}(A)$ have Chevalley generators $e_0,\ldots,e_n$ and $f_0,\ldots,f_n$ and a center $\mathbb{C}c$. Since $L(\Lambda)$ is irreducible we have $\pi(c)=m\,\mathrm{Id}$, where π denotes the representation of $\mathbf{g}(A)$ on $L(\Lambda)$.

The principal grading δ is determined by

$$\delta(e_i)=-\delta(f_j)=1 \quad (i,j=0,\ldots,n).$$

Graded will always mean graded with respect to δ.

We suppose we are given a graded Heisenberg subalgebra $\mathbf{s}$ in $\mathbf{g}(A)$ with basis $\{p_i,q_j,c\}$ $(i,j\in I\subset\mathbb{N})$ such that

$$[p_i,q_j]=\delta_{ij}\cdot c \quad\text{and}\quad \delta(p_i)=-\delta(q_i)=i.$$

Moreover, we assume $-\omega_0(q_i)=a_i p_i$ $(a_i\in\mathbb{C})$, where ω_0 denotes the antilinear Cartan involution.

Let v_Λ denote the highest weight vector of $L(\Lambda)$. We define the grading δ_L on $L(\Lambda)$ by

$$\delta_L(\pi(g)\cdot w)=-\delta(g)+\delta_L(w),\quad \delta_L(v_\Lambda)=0 \qquad [w\in L(\Lambda),\ g\in\mathbf{g}(A)]. \tag{2.1}$$

The module $L(\Lambda)$ can be considered as an $\mathbf{s}$-module; it will split up in a direct sum of irreducible $\mathbf{s}$-modules all isomorphic to each other:

$$\begin{aligned} &L(\Lambda)\cong\bigoplus_{j\ge 0} R\otimes_{\mathbb{C}} u_j,\quad R=\mathbb{C}[x_i,\ i\in I],\\ &\pi(p_i)=m\frac{\partial}{\partial x_i}\otimes 1,\quad \pi(q_i)=x_i\otimes 1,\\ &\pi(c)=m\,\mathrm{Id}. \end{aligned} \tag{2.2}$$

Here $1\otimes u_j$ are the vacuum vectors of the irreducible components, all with eigenvalue m. We suppose $v_\Lambda\cong 1\otimes u_0$. The unique nondegenerate contravariant Hermitian form H_1 on $L(\Lambda)$ with $H_1(v_\Lambda,v_\Lambda)=1$ is very important for our purposes.

To construct τ-functions we consider the group G generated by $\exp(\pi(te_i))$ and $\exp(\pi(tf_i))$ $(i=0,\ldots,n,\ t\in\mathbb{C})$. The τ-function $\tau(g)$ is defined by

$$\tau(g)=g\cdot v_\Lambda \quad (g\in G).$$

To find equations satisfied by $\tau(g)$ one considers $L(\Lambda)\otimes L(\Lambda)$. This module is completely reducible. The module generated by $v_\Lambda\otimes v_\Lambda$ is denoted by L_{high} [and isomorphic to $L(2\Lambda)$] and the submodule $L_{\text{high}}^{\perp}$ by L_{low}. Here orthogonality is taken with respect to H defined by

$$H(v_1\otimes w_1,\ v_2\otimes w_2)=H_1(v_1,v_2)\cdot H_1(w_1,w_2). \tag{2.3}$$

Since $\tau(g)\otimes\tau(g)\in L_{\text{high}}$ we have

$$H\left(\sum v_i\otimes w_i,\ \tau(g)\otimes\tau(g)\right)=0 \quad \left(\sum v_i\otimes w_i\in L_{\text{low}}\right). \tag{2.4}$$

We write these equations out in the realization (2.2), omitting $\otimes_{\mathbb{C}}$ and setting $H_1(u_i,u_j)=\epsilon_{ij}$. For $v=\Sigma P_i(x)u_i$ and $w=\Sigma Q_i(x)u_i$ we have

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$$H_1(v,w) = H_1\left(\sum P_i(x)u_i,\ \sum Q_j(x)u_j\right)$$

$$= \sum_{i,j} \epsilon_{ij}\overline{P}_i(m\tilde{D}_x)Q_j(x)|_{x=0}, \tag{2.5}$$

where

$$\tilde{D}_x = \left(a_1\frac{\partial}{\partial x_1}, a_2\frac{\partial}{\partial x_2}, \cdots\right).$$

For $v \otimes w$ we write

$$v \otimes w = \sum_{i,j} P_i(x^{(0)})Q_j(x^{(1)})u_i \otimes u_j$$

and

$$\tau(g) \otimes \tau(g) = \sum_{k,l} \tau_k(x^{(0)})\tau_l(x^{(1)})u_k \otimes u_l.$$

Changing variables

$$2x_j = x_j^{(0)} + x_j^{(1)} \quad \text{and} \quad 2y_j = x_j^{(0)} - x_j^{(1)}$$

leads to

$$\pi \otimes \pi(p_i) = m\frac{\partial}{\partial x_i}, \quad \pi \otimes \pi(q_j) = 2x_j,$$
$$\pi \otimes \pi(c) = 2m\ \mathrm{Id}. \tag{2.6}$$

We define $\mathrm{Hir} = L_{\mathrm{low}} \cap \mathbb{C}[y]$. For $\Sigma_{ij} P_{ij}(y)u_i \otimes u_j \in \mathrm{Hir}$ we have because of (2.6)

$$Q(x)\sum P_{ij}(y)u_i \otimes u_j \in L_{\mathrm{low}} \quad \text{for all } Q(x) \in \mathbb{C}[x].$$

Substitution in (2.4), using (2.5), leads to

$$\sum_{i,j,k,l} \overline{P}_{ij}\left(\frac{m}{2}\tilde{D}_y\right)\tau_k(x+y)\tau_l(x-y)\epsilon_{ik}\cdot\epsilon_{jl}|_{y=0} = 0, \tag{2.7}$$

for $\Sigma_{i,j} P_{ij}(y)u_i \otimes u_j \in \mathrm{Hir}$. These are the so-called bilinear equations (equations in Hirota form, see Ref. 5) that we are after.

III. DESCRIPTION OF $A_2^{(1)}$ AND $A_2^{(2)}$

We describe a realization of the derived algebras of these two Kac–Moody algebras. Therefore we first consider $A_2 \cong \mathrm{sl}(3,\mathbb{C})$. As a base for it we take

$$E_1 = E_{1,2}, \quad E_2 = E_{2,3}, \quad E_0 = E_{3,1}, \quad H_1 = E_{1,1} - E_{2,2},$$

$$F_1 = E_{2,1}, \quad F_2 = E_{3,2}, \quad F_0 = E_{1,3}, \quad H_2 = E_{2,2} - E_{3,3}.$$

As usual the commutator is given by $[E_{ij},E_{kl}] = \delta_{jk}E_{il} - \delta_{li}E_{kj}$. We define the elements

$$M_1 = (i/\sqrt{3})(E_1 - E_2 + E_0)$$

and

$$M_2 = -i\sqrt{3}(F_1 - F_2 + F_0).$$

We have $[M_1,M_2] = 0$.

Further, we introduce with $\epsilon = \frac{1}{2} + \frac{1}{2}i\sqrt{3}$,

$$A_{10} = -H_1 + \epsilon^2 H_2, \quad A_{20} = -H_1 - \epsilon H_2,$$
$$A_{11} = -\epsilon E_0 - E_2 + \epsilon^2 E_1, \quad A_{21} = \epsilon^2 E_0 - E_2 - \epsilon E_1,$$
$$A_{12} = -F_2 + \epsilon^2 F_1 - \epsilon F_0, \quad A_{22} = -F_2 - \epsilon F_1 + \epsilon^2 F_0.$$

These elements satisfy

$$[M_k,A_{ij}] = \lambda_{ik}A_{i,j+1}, \quad \lambda_{11} = -\lambda_{21} = 1,$$
$$\lambda_{12} = -\lambda_{22} = 3.$$

We define $A_{ik} = A_{ik'}$ with $k' = k \pmod 3$, $k' \in \{0,1,2\}$. We get similar results for λ_{ik}. Now we can describe the realization of $A_2^{(1)}$ in the following way. Denote

$$L_0 = \langle H_1,H_2\rangle, \quad L_1 = \langle E_0,E_1,E_2\rangle,$$
$$L_2 = \langle F_0,F_1,F_2\rangle. \tag{3.1}$$

As a vector space we take $A_2^{(1)}$ to be isomorphic to

$$\bigoplus_{\substack{k\in\mathbb{Z}\\ i=0,1,2}} (L_i \otimes t^{3k+i}) \oplus \mathbb{C}\cdot c.$$

The Lie product is defined by

$$[g_1 \otimes t^k + \lambda_1 c, g_2 \otimes t^l + \lambda_2 c]$$
$$= [g_1,g_2] \otimes t^{k+l} + (k/6)\delta_{k,-l}\langle g_1,g_2\rangle_{\mathrm{tr}}\cdot c, \tag{3.2}$$

$\langle g_1,g_2\rangle_{\mathrm{tr}}$ denotes $\mathrm{tr}(g_1g_2)$, where g_1 and g_2 are considered elements from $\mathrm{sl}(3,\mathbb{C})$.

Now we introduce the elements

$$p_m = \begin{cases} M_1 \otimes t^m & (m = 1 \bmod 3), \\ M_2 \otimes t^m & (m = 2 \bmod 3), \end{cases}$$
$$q_m = \begin{cases} (1/m)M_2 \otimes t^{-m} & (m = 1 \bmod 3), \\ (1/m)M_1 \otimes t^{-m} & (m = 2 \bmod 3). \end{cases} \tag{3.3}$$

Denote $\mathbf{s} = \langle p_m,q_m,c\rangle$, $m \in I = \{i \in \mathbb{N} | i \neq 0 \bmod 3\}$. This is a Heisenberg subalgebra of $A_2^{(1)}$ with

$$[p_m,q_n] = \tfrac{1}{2}\delta_{m,n}c.$$

Introduce

$$A_j(z) = \sum_{k\in\mathbb{Z}} (A_{jk} \otimes t^k)z^{-k}.$$

This is not an element of the Lie algebra $A_2^{(1)}$, but the homogeneous terms in z are. One easily calculates the following brackets:

$$[p_m,A_j(z)] = \lambda_{jm}z^m A_j(z),$$
$$[q_m,A_j(z)] = (z^{-m}/m)\lambda_{j,-m}A_j(z). \tag{3.4}$$

Now it is easy to describe $A_2^{(2)}$ as a subalgebra of $A_2^{(1)}$. Introduce the following subspaces of $\mathrm{sl}(3,\mathbb{C})$:

$$V_0 = \langle H_1 + H_2\rangle, \quad V_1 = \langle E_1 - E_2,E_0\rangle,$$
$$V_2 = \langle F_1 + F_2\rangle, \quad V_3 = \langle H_1 - H_2\rangle, \tag{3.5}$$
$$V_4 = \langle E_1 + E_2\rangle, \quad V_5 = \langle F_1 - F_2,F_0\rangle.$$

As a vector space we take $A_2^{(2)}$ isomorphic to

$$\bigoplus_{\substack{k\in\mathbb{Z}\\ j=0,\ldots,5}} (V_j \otimes t^{6k+j}) \oplus \mathbb{C}\cdot c;$$

and the Lie product is taken as in (3.2).

After a calculation one finds

$$
\begin{aligned}
&H_1 + H_2 = (1/\sqrt{3})\epsilon^2 A_{10} + (i/\sqrt{3})\epsilon A_{20},\\
&H_1 - H_2 = \epsilon^2 A_{10} - \epsilon A_{20},\\
&E_1 - E_2 - E_0 + \tfrac{1}{3} i\sqrt{3} M_1 = -\tfrac{2}{3}\epsilon^2 A_{11} + \tfrac{2}{3}\epsilon A_{21},\\
&E_1 + E_2 = (i/\sqrt{3})\epsilon^2 A_{11} + (i/\sqrt{3})\epsilon A_{21},\\
&F_1 + F_2 = (i/\sqrt{3})\epsilon^2 A_{12} + (i/\sqrt{3})\epsilon A_{22},\\
&F_1 - F_2 - F_0 - \tfrac{1}{9} i\sqrt{3} M_2 = -\tfrac{2}{3}\epsilon^2 A_{12} + \tfrac{2}{3}\epsilon A_{22}.
\end{aligned}
\tag{3.6}
$$

IV. THE $A_2^{(1)}$-MODULES $L(\Lambda_i)$ AND EQUATIONS

Here $A_2^{(1)}$ has Chevalley generators $e_i = E_i \otimes t$, $f_i = F_i \otimes t^{-1}$ $(i = 0,1,2)$. We define $\alpha_i^v = [e_i, f_i]$, so

$$
\alpha_0^v = -(H_1 + H_2) \otimes 1 + \tfrac{1}{6} c,
$$

$$
\alpha_i^v = H_i \otimes 1 + \tfrac{1}{6} c \quad (i = 1,2).
$$

Now Λ_i is defined by $\Lambda_i(\Sigma \lambda_j \alpha_j^v) = \lambda_i$.

Here $L(\Lambda_i)$ is the unique irreducible graded highest weight module, with highest weight Λ_i. Here graded is taken with respect to δ_L of (2.1). Denoting the subspace of degree j by $L_j(\Lambda_i)$, we can calculate the q-dimension of $L(\Lambda_i)$ [cf. Proposition 10.10 (Ref. 3)],

$$
\begin{aligned}
\dim_q L(\Lambda_i) &= \sum_{j \geqslant 0} \dim L_j(\Lambda_i) q^j\\
&= \prod_{j \geqslant 0} (1 - q^{3j+1})^{-1} (1 - q^{3j+2})^{-1} =: s(q).
\end{aligned}
$$

Calculating the q-dimension in the realization (2.2), where $\mathbf{s}$ is taken as in Sec. III, we find

$$
\dim_q L(\Lambda_i) = \sum_{i \geqslant 0} s(q) q^{\delta_L(u_i)},
$$

so $L(\Lambda_i)$ remains irreducible considered as an $\mathbf{s}$-module. Therefore all Lie algebra elements can be represented as infinite order differential operators. Using the relations (3.4) we find

$$
\begin{aligned}
\pi_i(A_j(z)) = c_j(\Lambda_i) &\exp\left(\sum_{m \geqslant 1} \lambda_{im} z^m x_m \right)\\
&\times \exp\left(-\sum_{m \geqslant 1} \lambda_{i,-m} \frac{z^{-m}}{m} \frac{\partial}{\partial x_m} \right).
\end{aligned}
\tag{4.1}
$$

Moreover, since $\pi_i(A_{j0}) \cdot v_\Lambda = c_j(\Lambda_i) v_\Lambda$, we have $c_j(\Lambda_i) = \Lambda_i(A_{j0})$. One calculates that

$$
c_1(\Lambda_0) = -(i/\sqrt{3})\epsilon \quad \text{and} \quad c_2(\Lambda_0) = -(i/\sqrt{3})\epsilon^2.
$$

As explained in Sec. II, we now can introduce Hirota polynomials and τ-functions. Since $L(\Lambda_i)$ is irreducible as an $\mathbf{s}$-module we have

$$
\tau(x;g) = g \cdot v_{\Lambda_i} \in \mathbb{C}[x_1, x_2, x_4, \ldots].
$$

Usually we do not write g in $\tau(x;g)$. The first nontrivial equation in the form (2.7) is

$$
(D_1^4 - \tfrac{1}{9} D_2^2)(\tau(x) \cdot \tau(x)) = 0,
$$

where

$$
D^\alpha(\tau(x') \cdot \sigma(x)) := \frac{\partial^{|\alpha|}}{\partial y^\alpha} \tau(x' + y) \sigma(x - y) \Big|_{y=0}.
$$

Here α is a multi-index $(\alpha_1, \alpha_2, \ldots, \alpha_k)$ and $y^\alpha = y_1^{\alpha_1} \cdots y_k^{\alpha_k}$.

V. THE $A_2^{(2)}$-MODULE $L(\Lambda_1)$ AND EQUATIONS

In more detail we will perform the same construction for the basic module $L(\Lambda_1)$ of $A_2^{(2)}$. The realization that we will discuss can be found in Ref. 6. We use a different normalization to find equations in a nicer form. Here $A_2^{(2)}$ contains a maximal Heisenberg subalgebra $\tilde{\mathbf{s}}$ of the following form:

$$
\begin{aligned}
\tilde{p}_m &= [1/(\epsilon^m + 1)] T_m \otimes t^m,\\
\tilde{q}_m &= (2/m)(\epsilon^m + 1) T_{-m} \otimes t^{-m}\\
&\qquad (m = \pm 1 \bmod 6),
\end{aligned}
$$

where

$$
T_m = \begin{cases} E_0 + E_1 - E_2, & m = 1 \pmod 6,\\ F_0 + F_1 - F_2, & m = -1 \pmod 6. \end{cases}
$$

Note that $\mathbf{s} \cap A_2^{(2)} = \tilde{\mathbf{s}}$ and $\omega_0(\tilde{q}_m) = (6/m)\tilde{p}_m$. As Chevalley generators of $A_2^{(2)}$ we take

$$
\tilde{e}_0 = E_0 \otimes t, \quad \tilde{e}_1 = \sqrt{2}(E_1 - E_2),
$$

$$
\tilde{f}_0 = F_0 \otimes t^{-1}, \quad \tilde{f}_0 = \sqrt{2}(F_1 - F_2),
$$

we use $\tilde{}$ to distinguish these elements from the generators of $A_2^{(1)}$. We find

$$
\tilde{\alpha}_0^v = [\tilde{e}_0, \tilde{f}_0] = -(H_1 + H_2) \otimes 1 + \tfrac{1}{6} c,
$$

$$
\tilde{\alpha}_1^v = [\tilde{e}_1, \tilde{f}_1] = 2(H_1 + H_2) \otimes 1 + \tfrac{2}{3} c.
$$

Calculating the q-dimension of $L(\Lambda_1)$, one finds

$$
\dim_q L(\Lambda_1) = \prod_{j \geqslant 0} (1 - q^{6j+1})^{-1} (1 - q^{6j+5})^{-1} =: r(q).
$$

Since $r(q) = \Pi_{j \geqslant 1} (1 - q^j)^{-\dim \tilde{\mathbf{s}}_j}$, we see that $L(\Lambda_1)$ remains irreducible as an $\tilde{\mathbf{s}}$-module. The uniqueness of highest weight modules of Heisenberg algebras then gives that we can assume that the action $\tilde{\pi}$ of $\tilde{p}_m$ and $\tilde{q}_m$ is

$$
\tilde{\pi}(\tilde{p}_m) = \frac{\partial}{\partial x_m}, \quad \tilde{\pi}(\tilde{q}_m) = x_m, \quad \tilde{\pi}(c) = \mathrm{Id},
$$

and

$$
L(\Lambda_1) \cong \mathbb{C}[x_1, x_5, x_7, \ldots].
\tag{5.1}
$$

To extend this representation $\tilde{\pi}$ to all of $A_2^{(2)}$ we introduce

$$
A = \begin{pmatrix} -1 & 1 & 1\\ -\epsilon & \epsilon & \epsilon\\ \epsilon^2 & -\epsilon^2 & -\epsilon^2 \end{pmatrix} \in \mathrm{sl}(3,\mathbb{C}).
$$

We can split up A in homogeneous components with respect to the grading of (3.5). We then find $A = \Sigma_{j=0}^5 A_j$, where

$$
\begin{aligned}
A_0 &= \tfrac{1}{2} i\sqrt{3}\epsilon(H_1 + H_2),\\
A_1 &= -\tfrac{3}{4}\epsilon^2(E_1 - E_2 - E_0 + \tfrac{1}{3} i\sqrt{3} M_1),\\
A_2 &= -\tfrac{1}{2} i\sqrt{3}(F_1 + F_2),\\
A_3 &= -\tfrac{1}{2}\epsilon(H_1 - H_2),\\
A_4 &= -\tfrac{1}{2} i\sqrt{3}\epsilon^2(E_1 + E_2),\\
A_5 &= -\tfrac{3}{4}(F_1 - F_2 - F_0 - \tfrac{1}{9} i\sqrt{3} M_2).
\end{aligned}
\tag{5.2}
$$

Introducing

$$
A(z) = \sum_{j \in Z} (A_j \otimes t^j) z^{-j} \quad (A_j = A_{j \bmod 6}),
$$

we find

$$[p_m, A(z)] = z^m A(z), \quad [q_m, A(z)] = (6/m) z^{-m} A(z),$$

so

$$\tilde{\pi}(A(z)) = a \cdot \exp\left(\sum_{m>1} z^m x_m\right) \exp\left(-\sum_{m>1} \frac{6}{m} z^{-m} \frac{\partial}{\partial x_m}\right),$$

where the sums are only taken for $m = \pm 1 \pmod 6$. From the formula one finds

$$\tilde{\pi}(A_{-j} \otimes t^{-j}) = a \sum_l p_{j+l}(x_m) p_l\left(-\frac{6}{m} \frac{\partial}{\partial x_m}\right).$$

Here $p_k(x)$ denote the Schur polynomials defined by

$$\exp\left(\sum_{l>1} x_l z^l\right) = \sum p_k(x) z^k.$$

Since $A_0 \otimes 1 = (i\sqrt{3}/12)\epsilon(\tilde{\alpha}_1^v - 4\tilde{\alpha}_0^v)$ we find $\tilde{\pi}(A_0 \otimes 1) \cdot 1 = a \cdot 1 = (i\sqrt{3}/12)\epsilon$.

Now we can turn to the construction of the equations. We introduce the module $L(\Lambda_1) \otimes L(\Lambda_1)$ and the action $\tilde{\pi} \otimes \tilde{\pi}$ by

$$(\tilde{\pi} \otimes \tilde{\pi})(g)(v \otimes w) = \tilde{\pi}(g) v \otimes w + v \otimes \tilde{\pi}(g) w.$$

The grading δ_L is extended by $\delta_L(v \otimes w) = \delta_L(v) + \delta_L(w)$. We work in the realization (5.1), and an element $P(x) \otimes Q(x)$ will be written as $P(x^{(0)}) Q(x^{(1)})$.

Introducing

$$\tilde{x}_j = \tfrac{1}{2}(x_j^{(0)} + x_j^{(1)}) \quad \text{and} \quad y_j = \tfrac{1}{2}(x_j^{(0)} - x_j^{(1)}),$$

one finds

$$(\tilde{\pi} \otimes \tilde{\pi})(\tilde{p}_j) = \frac{\partial}{\partial \tilde{x}_j},$$

$$(\tilde{\pi} \otimes \tilde{\pi})(\tilde{q}_j) = 2\tilde{x}_j, \quad (\tilde{\pi} \otimes \tilde{\pi})(c) = 2\,\mathrm{Id}.$$

Moreover

$$(\tilde{\pi} \otimes \tilde{\pi})(A_{-j} \otimes t^{-j})$$

$$= a \left\{ \sum_l p_{j+l}(\tilde{x}_m + y_m) p_l\left(-\frac{3}{m}\left(\frac{\partial}{\partial \tilde{x}_m} + \frac{\partial}{\partial y_m}\right)\right) + \sum_l p_{j+l}(\tilde{x}_m - y_m) p_l\left(-\frac{3}{m}\left(\frac{\partial}{\partial \tilde{x}_m} - \frac{\partial}{\partial y_m}\right)\right)\right\}.$$

Denote by L_{high} the $A_2^{(2)}$-submodule generated by $v_{\Lambda_1} \otimes v_{\Lambda_1} = 1$ and $L_{\text{low}} = L_{\text{high}}^{\perp}$. Here $\perp$ is taken with respect to H defined by (2.3) and (2.5). Note that in this case $u_i = 0$ $(i \geq 1)$, so $\epsilon_{ij} = \delta_{ij} \cdot \delta_{i0}$. Moreover, $a_i = 6/i$ and $m = 1$.

We calculate the interesting q-dimensions. We know

$$\dim_q [L(\Lambda_1) \otimes L(\Lambda_1)] = \{\dim_q L(\Lambda_1)\}^2 = r^2(q).$$

Since $L_{\text{high}} \cong L(2\Lambda_1)$ we find using Proposition 10.10 from Ref. 3,

$$\dim_q L_{\text{high}} = \prod_{j>1} (1 - q^j)^{-1} \cdot \prod_{j>0} (1 - q^{10j+4})(1 - q^{10j+6}) \times (1 - q^{10j+10})(1 - q^{6j+3}).$$

Since $L(\Lambda_1) \otimes L(\Lambda_1) = L_{\text{high}} \oplus L_{\text{low}}$ we have

$$\dim_q L_{\text{low}} = r^2(q) - \dim_q L_{\text{high}}.$$

Finally, $L_{\text{low}} = \text{Hir} \otimes \mathbb{C}[\tilde{x}]$, so we find

$$\dim_q \text{Hir} = r(q) - r^{-1}(q) \dim_q L_{\text{high}}$$

$$= r(q) - \prod_{j>0} (1 - q^{10j+z})^{-1} (1 - q^{10j+8})^{-1}$$

$$= q + q^3 + 2q^5 + q^6 + \cdots$$

$$= \dim_q \mathbb{C}[y] - \dim_q \Omega,$$

where $\Omega = L_{\text{high}} \cap \mathbb{C}[y]$ represents the space of constraints. Since we have only odd variables we have only nontrivial equations for elements of Hir with even degree (see Ref. 5). So the first nontrivial equation is of degree 6. Here there is one constraint. Calculating

$$(\tilde{\pi} \otimes \tilde{\pi})(A_{-6} \otimes t^{-6}) \cdot 1 = a\{p_6(\tilde{x}_m + y_m) + p_6(\tilde{x}_m - y_m)\}$$

one finds $\Omega_6 = \langle (1/6!) y_1^6 + y_1 y_5 \rangle$.

Suppose $\bar{\alpha} y_1^6 + \bar{\beta} y_1 y_5 \in \text{Hir}$, then we know

$$H(\bar{\alpha} y_1^6 + \bar{\beta} y_1 y_5, (1/6!) y_1^6 + y_1 y_5) = 0$$

$$\Rightarrow \alpha \cdot (\tfrac{1}{2})^6 6^6 + \beta (\tfrac{1}{2})^2 \cdot 6 \cdot \tfrac{6}{5} = 0.$$

From this one finds

$$(D_1^6 - D_1 D_5)(\tau(\tilde{x}) \cdot \tau(\tilde{x})) = 0.$$

VI. THE $A_2^{(2)}$-MODULE $L(\Lambda_0)$ AND EQUATIONS

We can consider the $A_2^{(1)}$-module $L(\Lambda_0)$ as an $A_2^{(2)}$-module. The submodule L generated by $V_{\Lambda_0} \in L(\Lambda_0)$ is irreducible, which one can prove using the grading and the Hermitian form H_1 on $L(\Lambda_0)$. One easily calculates

$$\pi_0\left(\sum \lambda_i \tilde{\alpha}_i^v\right) \cdot v_{\Lambda_0} = \lambda_0 \cdot v_{\Lambda_0},$$

so $L \cong L(\Lambda_0)$ as an $A_2^{(2)}$-module. From now on we mean this $L(\Lambda_0)$, if we write $L(\Lambda_0)$. Since $L(\Lambda_0) \cong L$, $L(\Lambda_0)$ can be realized as a subspace of $\mathbb{C}[x_i, i \neq 0 \bmod 3]$. We also can write down the explicit form of the action of elements of $A_2^{(2)}$ by using (3.6) and (4.1), and in particular

$$\pi_0(p_m) = \frac{\partial}{\partial x_m}, \quad \pi_0(q_m) = x_m \quad (m = \pm 1 \bmod 6).$$

We consider $L(\Lambda_0)$ as an $\tilde{\mathfrak{s}}$-module. Since

$$\dim_q L(\Lambda_0) = r(q) \prod_{j>0} (1 - q^{10j+4})^{-1} (1 - q^{10j+6})^{-1}$$

$$= r(q)\{1 + q^4 + q^6 + \cdots\},$$

we see that $L(\Lambda_0)$ does not remain irreducible as an $\tilde{\mathfrak{s}}$-module. We introduce therefore $u_0 = 1$, $u_1 = x_2^2$, $u_2 = x_2 x_4, \ldots$. As before we define L_{high} in $L(\Lambda_0) \otimes L(\Lambda_0)$ and Hir. Since $L_{\text{high}} \cong L(2\Lambda_0)$ we find

$$\dim_q L_{\text{high}} = r(q) \prod_{j>0} (1 - q^{10j+2})^{-1} (1 - q^{10j+8})^{-1}$$

and

$$\dim_q \mathrm{Hir} = r(q)\prod_{j>0}(1-q^{10+4})^{-2}(1-q^{10j+6})^{-2}$$
$$-\prod_{j>0}(1-q^{10j+2})^{-1}(1-q^{10j+8})^{-1}$$
$$= q + q^3 + 2q^4 + 3q^5 + 4q^6 + \cdots .$$

Again we have $\Omega = \mathbb{C}[y]\cap L_{\text{high}}$.

Analyzing Hir in graded subspaces Hir_j we find for $j = 1,3,5$ only elements leading to trivial equations, for example, $\mathrm{Hir}_3 = \langle y_1^3 u_0 \otimes u_0\rangle$. For $j = 4$ there is one constraint and one nontrivial equation. Calculating

$$(\pi_0\otimes\pi_0)((f_1+f_2)\otimes t^{-4})1\otimes 1$$

we find $\omega_4 = \frac{1}{6}y_1^4 u_0\otimes u_0 + 9(u_1\otimes u_0 + u_0\otimes u_1)\in\Omega$, which leads to the equation

$$D_1^4(\tau_0(x)\cdot\tau_0(x)) - \tfrac{4}{9}\tau_0(x)\cdot\tau_1(x) = 0. \tag{6.1}$$

For degree 6 there are two nontrivial equations, of which one contains only τ_0 and τ_1. There are also two constraints

$$\omega_6 = \tfrac{1}{180}y_1^6 u_0\otimes u_0 + \tfrac{9}{2}y_1^2(u_1\otimes u_0 + u_0\otimes u_1)$$
$$+ 12y_1y_5 u_0\otimes u_0 + 6(u_2\otimes u_0 + u_0\otimes u_2),$$
$$\omega_6' = \tfrac{1}{6}y_1^6 u_0\otimes u_0 - 9y_1^2(u_1\otimes u_0 + u_0\otimes u_1)$$
$$+ 36(u_2\otimes u_0 + u_0\otimes u_2).$$

We find

$$(D_1^6 - \tfrac{16}{3}D_1D_5)(\tau_0(x)\cdot\tau_0(x)) + \tfrac{20}{3}D_1^2(\tau_0(x)\cdot\tau_1(x)) = 0. \tag{6.2}$$

VII. SPECIAL TYPE OF MODIFIED EQUATIONS

We have constructed two $A_2^{(2)}$-modules $L(\Lambda_0)$ and $L(\Lambda_1)$, in a realization in which the Heisenberg algebra $\tilde{\mathfrak{s}}$ acts canonically. We can now consider $L(\Lambda_0)\otimes L(\Lambda_1)$ to find equations connecting the two hierarchies found before. Note that $L(\Lambda_0)$ is reducible and $L(\Lambda_1)$ is irreducible as an $\tilde{\mathfrak{s}}$-module. We denote $u_0\in L(\Lambda_1)$ by u, and also $\tau_0(x)$ by $\tau(x)$. Since

$$\dim_q L(\Lambda_0+\Lambda_1)$$
$$= r(x)\prod_{j>0}(1-q^{2j+1})^{-1}(1-q^{12j+2})(1-q^{12j+10})$$

we have

$$\dim_q \mathrm{Hir} = r(q)\prod_{j>0}(1-q^{10j+4})^{-1}(1-q^{10j+6})^{-1}$$
$$-\prod_{j>0}(1-q^{2j+1})^{-1}(1-q^{12j+2})$$
$$\cdot(1-q^{12j+10})$$
$$= \sum_{i>0}\dim_q \mathbb{C}[y]u_i\otimes u - \dim_q\Omega$$
$$= (q^2 + q^4 + 2q^5 + \cdots).$$

Recall the elements p_m, q_m ($m = \pm 1 \bmod 6$) introduced in (3.3). Their action in $L(\Lambda_0)\otimes L(\Lambda_1)$ is

$$(\pi_0\otimes\tilde{\pi})(p_m) = \frac{\partial}{\partial x_m^{(0)}} + \alpha_m\frac{\partial}{\partial x_m^{(1)}},$$
$$(\pi_0\otimes\tilde{\pi})(q_m) = x_m^{(0)} + \beta_m x_m^{(1)},$$

where

$$\alpha_m = (i/\sqrt{3})(\epsilon+1) \quad (m = 1 \bmod 6),$$
$$\alpha_m = i\sqrt{3}(\epsilon^2-1) \quad (m = -1 \bmod 6),$$

and

$$\beta_m = 1/2\alpha_m.$$

Now define the elements x_m and y_m by

$$x_m = \tfrac{1}{3}(x_m^{(0)} + \beta_m x_m^{(1)}), \quad y_m = \tfrac{1}{3}(x_m^{(0)} - 2\beta_m x_m^{(1)}),$$

then

$$(\pi_0\otimes\tilde{\pi})(p_m) = \frac{1}{2}\frac{\partial}{\partial x_m} \quad \text{and} \quad (\pi_0\otimes\tilde{\pi})(q_m) = 3x_m.$$

Now we can calculate the constraints and the Hirota polynomials. For degree 2 there are nonzero elements in $\mathbb{C}[y]\cap L_{\text{high}}$, so we find

$$y_1^2 u_0\otimes u\in\mathrm{Hir}$$

and

$$D_1^2(\tau_0(2x)\cdot\tau(x)) = 0,$$

where $\tau(x) = \tau(\beta\cdot\tilde{x})$, $\beta = (\beta_1,\beta_2,\ldots)$, and $\tau(\beta\tilde{x}) = \tau(\beta\tilde{x};g)$ as defined in Sec. II.

For degree 4 we have to calculate the highest order part of

$$(\pi_0\otimes\tilde{\pi})((f_1+f_2)\otimes t^{-4})(u_0\otimes u)$$

yielding

$$\Omega_4 = \langle(1/4!)y_1^4 u_0\otimes u - \tfrac{3}{2}u_1\otimes u\rangle$$

leading to

$$D_1^4(\tau_0(2x)\cdot\tau(x)) + \tfrac{2}{3}\tau_1(2x)\tau(x) = 0,$$

which is a consequence of (7.1) and (6.1).

Finally, calculating

$$(\pi_0\otimes\tilde{\pi})((e_1 - e_2 - e_0 + \tfrac{1}{3}i\sqrt{3}M_1)\otimes t^{-5})(u_0\otimes u)$$

leads to

$$\Omega_5 = \langle\tfrac{1}{10}y_1^5 u_0\otimes u + 6y_1u_1\otimes u + 6y_5u_0\otimes u\rangle$$

yielding one equation in τ_0 and τ,

$$(D_1^5 - 2D_5)(\tau_0(2x)\cdot\tau(x)) = 0.$$

VIII. DISCUSSION

In Secs. IV–VI we found three hierarchies of equations. The first one (in Sec. IV) is the well-known Boussinesq hierarchy and needs no further discussion.

The second hierarchy (Sec. V) is a hierarchy of which the first equation is the Sawada–Kotera equation

$$u_t = (u_{xxxx} + 15uu_{xx} + 15u^3)_x,$$

$$u = \partial_{xx}\log\tau, \quad t = \tilde{x}_5, \quad x = \tilde{x}_1.$$

The construction given here corresponds to reduction to $A_2^{(2)}$ of the BKP hierarchy (cf. Ref. 2). One also gets this equation by considering $L(2\Lambda_1)\otimes L(2\Lambda_1)$ (cf. §8 and Table 4 of Ref. 2).

The third hierarchy (Sec. VI) has as its first equation the Kaup equation (see also §8 and Table 4 of Ref. 2),

$$\tfrac{1}{3}u_t = (u_{xxxx} + 15uu_{xx} + 15u^3 + \tfrac{45}{4}u_x^2)_x = 0,$$
$$u = \partial_{xx}\log\tau_0, \quad t = x_5, \quad x = x_1.$$

Here we see the explanation of the substitutions

$$\tau_0\Big|_{x_2 = x_4 = \ldots = 0} \quad \text{and} \quad \frac{\partial}{\partial x_2^2}\tau_0\Big|_{x_2 = x_4 = \ldots = 0}$$

in Ref. 2, where τ_0 is the τ-function of the KP hierarchy. In our context these variables are not real variables as they do not occur in the Heisenberg algebra $\tilde{\mathfrak{s}}$.

In Sec. VIII we find a transformation connecting those two hierarchies. Setting

$$v(x) = \partial_x \log(\tau_0(2x)/\tau^2(x))$$

we have

$$\tfrac{16}{3}v_t = (v_{xxxx} + 5v_{xx}v_x - 5v_{xx}v^2 - 5v_x^2 v + v^5)_x, \quad (8.1)$$

an equation also occurring in Table 4 of Ref. 2, but here found as a relation between the hierarchies of $L(\Lambda_0)$ and $L(2\Lambda_1)$. In view of the relation (6.7) of Ref. 2, the square in (8.1) need not surprise us.

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On the prolongation approach in three dimensions for the conservation laws and Lax pair of the Benjamin–Ono equation

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The prolongation structure approach of Wahlquist and Estabrook [J. Math. Phys. **16**, 1 (1975)] is used effectively in a new situation in relation to the integrodifferential type BO equation (the Benjamin–Ono equation). The main clue lies in the possible differential equation representation of such equations in three dimensions. Here it is shown how the usual analysis of prolongation structure can be utilized to deduce a Lax pair for a BO type equation in three dimensions. Effectiveness of the present approach is further demonstrated by an independent derivation of some conservation laws associated with the equation. Last, the whole formalism is reduced to two dimensions to make contact with known results.

I. INTRODUCTION

Very recently, it has been demonstrated by Grammaticos *et al.*[1] that a purely differential type representation is possible for a Benjamin–Ono (BO) type[2] integrodifferential equation by introducing a new independent variable y as any extra space coordinate. On the other hand, it is possible to revert to the usual integral form of the BO equation by solving the auxiliary equation on the boundary $y=0$. These authors felt the need for such a representation when they tried to make a Painléve test for the BO equation. Here we show that such a representation in three dimensions can be further utilized to derive the IST equation of the BO equation by following the methodologies of Wahlquist and Estabrook.[3] The technique of Wahlquist and Estabrook was extended to three dimensions by Morris.[4] Here we give a generalized form of prolongation analysis in many dimensions and then apply the technique to our case. The method is quite effective in yielding the Lax pair and the conservation laws related to the BO equation. In the last section we show how to go back to the physical two-dimensional space, by using the ansatz of Grammaticos *et al.*

II. FORMULATION

The BO equation is written as

$$u_t + uu_x + \frac{p}{\pi}\int \frac{u_{x'x'}(x')}{x'-x}\,dx' = 0\,. \tag{1}$$

It has been proved in Ref. 1 that Eq. (1) is equivalent to the following set in three dimensions:

$$u_{xx} + u_{yy} = 0\,, \quad u_t + uu_x + u_{xy} = 0, \tag{2}$$

under proper boundary conditions. The integral term reappears if we solve the first equation of (2) by the Green's function approach and substitute in the second equation of (2). To proceed with the prolongation analysis in three dimensions we define the independent variables

$$u_x = p, \quad u_y = r\,. \tag{3}$$

Then the following three forms are seen to be equivalent to (1) under proper sectioning:

$$\begin{aligned}
\alpha_1 &= du\wedge dy\wedge dt - p\,dx\wedge dy\wedge dt\,,\\
\alpha_2 &= -du\wedge dx\wedge dt - r\,dx\wedge dy\wedge dt\,,\\
\alpha_3 &= dp\wedge dy\wedge dt - dr\wedge dx\wedge dt\,,\\
\alpha_4 &= dr\wedge dy\wedge dt + up\,dx\wedge dy\wedge dt + du\wedge dx\wedge dy\,.
\end{aligned} \tag{4}$$

Here we first indicate the necessary steps for the prolongation analysis in higher dimension in complete generality and then apply them to the set (4). In n dimensions we can summarize by stating the following.

(i) If the nonlinear equations are equivalent to the differential forms $\alpha_1, \alpha_2, \ldots, \alpha_n$, all (n) forms

$$\alpha^A = (1/n!)\alpha^A_{\mu_1\mu_2\cdots\mu_n}\,dx^{\mu_1}\wedge dx^{\mu_2}\wedge\cdots\wedge dx^{\mu_n}\,. \tag{5}$$

(ii) They satisfy the closer condition

$$d\alpha^A \subset I, \quad I=\{\alpha^A\}\,. \tag{6}$$

(iii) Then if we introduce the prolongation variables y's and the $(n-1)$ forms

$$\Omega^i = \beta^i_j\wedge\omega^j, \quad i=1,2,3,\ldots,\dim y^j\,, \tag{7}$$

the $\beta^i{}_j$ are $(n-2)$ forms to be determined:

$$\beta^i{}_j = \frac{1}{(n-2)!}b^i{}_{i\mu_1\mu_2\cdots\mu_{n-2}}\,dx^{\mu_1}\wedge dx^{\mu_2}\cdots\wedge dx^{\mu_{n-2}}\,, \tag{8}$$

with ω^i the connection one-form defined as

$$\omega^i = dy^i + \sum \wedge^{ik}\,dx^K\,. \tag{9}$$

(iv) We now then again impose the closer condition on the extended set $I' = \{\alpha^i, \Omega^i\}$ in the form $d\Omega^i \subset I'$, which will fix up the corresponding structure of the prolongation algebra. In our case, these equations are specialized as follows:

$$\omega^i = dy^i + F^i\,dx + G^i\,dy + H^i\,dt\,, \tag{10}$$

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where F^i, G^i, and H^i depend on (u,p,r,x,y,t,y_i) and

$$\Omega^j = (a_K^j\,dx + b_K^j\,dy + c_K^j\,dt)\wedge\omega^K, \tag{11}$$

where a_K^j, b_K^j, and c_K^j are constants matrices satisfying the commutation rules

$$[a_\alpha^i, b_\alpha^i] = 0, \quad [b_K^j, c_K^j] = 0, \quad [c_{\alpha'}^j, a_{\beta'}^j] = 0. \tag{12}$$

From (9) and (10) we obtain

$$\Omega^j = a_K^j\,dx\wedge dy^K + b_K^j\,dy\wedge dy^K + c_K^j\,dt\wedge dy^K + L^j\,dx\wedge dy + M^j\,dt\wedge dx + N^j\,dt\wedge dy, \tag{13}$$

with

$$\begin{aligned} L^j &= aG^j - bF^j,\\ M^j &= cF^j - aH^j,\\ N^j &= cG^j - bH^j. \end{aligned} \tag{14}$$

Hence we have by exterior differentiation

$$d\Omega^j = L_{\sigma\mu}^j\,d\sigma_\mu\wedge dx\wedge dy + M_{\sigma\mu}^j\,d\sigma_\mu\wedge dt\wedge dx + N_{\sigma\mu}^j d\sigma_\mu\wedge dt\wedge dy. \tag{15}$$

Here, σ_μ stands for the set

$$\sigma_\mu \equiv \{x,y,t,y_K,u,p,r\}.$$

We now demand

$$d\Omega^j = \sum \alpha_i f_i^j + (\lambda\,dx + \mu\,dy + \nu\,dt)\wedge\Omega^j. \tag{16}$$

Equating coefficients of different three-forms $dp\wedge dy\wedge dt$, $dr\wedge dx\wedge dt$, etc., we get

$$\nu a^j - \lambda c^j = M_y, \quad \nu b^j - \eta c^j = N_y, \quad \lambda b^j - \eta a^j = L_y. \tag{17}$$

Furthermore, we have

$$N_p = -M_r, \quad N_r = -L_u,$$

along with

$$pN_u - rM_u - upN_r = \lambda N - \eta M - \nu L + L_t + M_y - N_x. \tag{18}$$

Now as in the case of two-dimensional theory we demand that our prolongation equations will be independent of explicit coordinate dependence. So the above equations reduce to

$$pN_u - rM_u - upN_r = \lambda N - \eta M - \nu L. \tag{19}$$

We now make an interesting observation that one can make a possible choice of the form

$$\lambda = -F_{y_K}, \quad \nu = -H_{y_K}, \quad \eta = -G_{y_K},$$

so that

$$\lambda N - \eta M - \nu L = NM_{y_K} - MN_{y_K} = [N, M]. \tag{20}$$

Hence finally our equations are

$$\begin{aligned} &N_p = -M_r, \quad N_r = -L_u,\\ &pN_u - rM_u - upN_r = [N, M]. \end{aligned} \tag{21}$$

Then the inverse scattering equations pertaining to the set are

$$\begin{aligned} &\xi_x = -M\xi - a\xi_t, \quad \xi_y = -N\xi - b\xi_t,\\ &a\xi_y - b\xi_x = -L_\xi. \end{aligned} \tag{22}$$

It is now necessary to impose some conditions on the matrices a and b as done by Morris.[4] In our case these conditions are

$$[a, b] = 0, \quad [N, a] + [b, M] = 0. \tag{23}$$

Let us now set

$$\begin{aligned} M &= x_1(y_i) + x_2(y_i)u + x_3(y_i)r,\\ N &= x_4(y_i) - x_3(y_i)p + x_5(y_i)u + x_6(y_i)u^2 + x_7(y_i)r \end{aligned} \tag{24}$$

in Eq. (21) to get

$$\begin{aligned} &[x_1, x_3] = -x_5, \quad [x_3, x_5] = 0,\\ &[x_2, x_3] = x - 2x_7, \quad [x_3, x_6] = 0,\\ &[x_3, x_4] + [x_1, x_7] = -x_2, \quad [x_3, x_7] = 0,\\ &[x_1, x_5] + [x_2, x_4] = 0, \quad [x_1, x_4] = 0,\\ &[x_1, x_6] + [x_2, x_5] = 0, \quad [x_2, x_6] = 0, \end{aligned} \tag{25}$$

which is the resultant incomplete Lie algebra. Now to close (25) we make the identification

$$x_5 = Kx_3, \quad x_7 = 2x_6.$$

Then the above set of commutators will reduce to

$$\begin{aligned} &[x_1, x_3] = -Kx_3, \quad [x_2, x_4] = K^2x_3,\\ &[x_2, x_3] = 0, \quad [x_1, x_6] = 0,\\ &[x_3, x_4] = 0, \quad [x_2, x_6] = 0,\\ &[x_1, x_4] = 0, \quad [x_3, x_6] = 0, \end{aligned} \tag{26}$$

since their use of Jacobi identities yields

$$[x_1, x_2] = -Kx_2; \quad [x_4, x_6] = x_6.$$

So we have obtained a closed 5×5 Lie algebra whose explicit realization in the regular representation[5] yields a Lax pair with 5×5 matrices, if we can solve Eq. (23) for a and b. First, we note that the matrices M and N have the form

$$M = \begin{pmatrix} 0 & 0 & 0 & 0 & 0\\ Ku & -K & 0 & -r & 0\\ Kr & 0 & -K & K^2u & 0\\ 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad N = \begin{pmatrix} 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 1 & p-Ku & 0\\ K^2u - Kp & -K^2 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & -(u^2+2r) & 1 \end{pmatrix}. \tag{27}$$

When this M and N are used in (23) we obtain

$$a=\begin{pmatrix}0&0&0&0&0\\0&0&0&0&0\\0&0&0&0&0\\0&0&0&0&0\\0&0&0&0&1\end{pmatrix}, \tag{28}$$

$b=5\times5$ unit matrix, so the Lax equations in three dimensions can be explicitly written as

$$\begin{aligned}&\xi^1_x=0,\quad \xi^2_x=-Ku\xi^1+K\xi^2+r\xi^4,\\&\xi^3_x=-Kr\xi^1+K\xi^3-K^2u\xi^4,\\&\xi^4_x=0,\quad \xi^5_x=\xi^5_t,\end{aligned} \tag{29}$$

and

$$\begin{aligned}&\xi^1_y=\xi^1_t,\quad \xi^2_y=-\xi^3-(p-Ku)\xi^4+\xi^2_t,\\&\xi^3_y=-(K^2u-Kp)\xi'+K^2\xi^2+\xi^3_t,\\&\xi^4_y=\xi^4_t,\quad \xi^5_y=(u^2+2r)\xi^4-\xi^5.\end{aligned} \tag{30}$$

Now a transition to the usual space-time variable of (x,t) is made if we use $U_y=TU_x$ or $rf=T_p$ and eliminate the redundant ξ_i's.

III. CONSERVATION LAWS

We now again call back our prolongation equations (19) and (21) to show that the independent derivation of some conservation laws can be made in our present formalism which were previously obtained by Chen and Lee.[6]

Let us for the time being drop the prolongation variables ξ_i's and keep the (x,y,t) dependence. Then Eqs. (18) are changed to

$$\begin{aligned}&N_p=-M_r,\quad N_r=-L_u,\\&pN_u-rM_u-upN_r=0=L_t+M_y-N_x.\end{aligned} \tag{31}$$

Now a conservation law in three dimensions is of the form

$$\frac{\partial L}{\partial t}+\frac{\partial M}{\partial y}+\frac{\partial(-N)}{\partial x}=0, \tag{32}$$

with L the density and M, $(-N)$ the components of currents, so that different conservation laws correspond to different solutions of (31) satisfying (32). It is not very difficult to show that one such solution set is given as

$$\begin{aligned}&L=-2\bar\alpha_1u+\bar\alpha_2,\quad M=\bar\alpha_3+\bar\alpha_4u_y,\\&N=\bar\alpha_5-\bar\alpha_4u_x+(u^2+2u_y)\bar\alpha_1,\end{aligned} \tag{33}$$

where $\bar\alpha_i$ are arbitrary constants. To generate more such conservation laws we follow the usual trick of demanding the closer of $d\Omega$ even when we consider some derived consequences of equation set (2). To illustrate the method we consider x derivative of (2), that is,

$$\begin{aligned}&u_{xxx}+u_{xyy}=0,\\&u_{xt}+u_x^2+u_xu_{xx}+u_{xxy}=0,\end{aligned} \tag{34}$$

which are equivalent to the following sets of differential forms:

$$\begin{aligned}&\alpha_5=-dr\wedge dx\wedge dt-s\,dx\wedge dy\wedge dt,\\&\alpha_6=dq\wedge dy\wedge dt+ds\wedge dy\wedge dt,\\&\alpha_7=-dq\wedge dx\wedge dt+(u+p^2)dx\wedge dy\wedge dt\\&\qquad+dp\wedge dx\wedge dy,\end{aligned} \tag{35}$$

with $U_{yy}=s$.

If we now demand

$$d\Omega=\sum_{i=1}^{7}f_i\alpha_i,$$

then we obtain

$$\begin{aligned}&L=\tilde\alpha_2u+\tilde\alpha_4u_x+\tilde\alpha_5,\\&M=\tilde\alpha_2u_x+\tilde\alpha_4u_{xx}+\tilde\alpha_9,\\&N=-\tilde\alpha_8u_{xx}-\tilde\alpha_4uu_x-\tfrac12\tilde\alpha_2u^2-\tilde\alpha_8u_{yy}.\end{aligned} \tag{36}$$

The two-dimensional form of the conservation laws can also be obtained by the same prescription as noted before.

In the above analysis we have indicated a methodical application of prolongation theory to the partial differential equation involving integral terms. The method is extensible to similar other completely integrable equations.

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Generalized complex superspace—Involutions of superfields

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Distinguished involutions called transposition and conjugation in the algebra of complex supernumbers are introduced. On the base of these involutions an analysis is developed over complex superspaces. Consistency of integration under supertransformations between two complex superspaces is shown.

I. INTRODUCTION

In our previous paper[1] we studied analyses of functions defined on generalized superspace, that is, differentiation and integration of functions in σ-commutative variables. There we treated only the real superspace over a real σ-commutative algebra, where the values of the sign function σ are constrained to ± 1. Over the complex field the values of σ are, in general, nth roots of 1 and therefore it is important to consider the complex superspace to treat functions in variables with general σ commutativity. And, of course, complex superspace plays an essential role in quantum field theory (Berezin[2]).

To develop an analysis on a complex superspace over a σ-commutative algebra A, it is necessary to define suitable involutions (conjugation $^-$ and transposition *) in A. The involutive structure of complex superspace induced by the transposition * makes it possible to define differentiation and integration of superfields in a similar fashion as we did in the real superspace. And, moreover, Taylor's expansion and the standard expansion formulas take more convenient forms in terms of transposition on complex superspace.

A striking aspect of our theory is a consistency theorem that asserts that the measures of superspaces are adjusted by the superdeterminant of the Jacobian matrix of a mapping between two spaces indexed by, in general, different index sets. In the real case, the consistency in this sense holds only within the same superspace (see Ref. 1).

In Sec. II we study involutions in σ-commutative algebras in general, and introduce a special involution * called the transposition on the algebra of complex supernumbers. By finding an appropriate factor system we can define another involution $^-$ called the conjugation associated with *.

In Sec. III we introduce the complex superspace with involutive structure induced from * and $^-$ given in Sec. II. We study differentiable functions (G^∞ functions) on complex superspace Z along the method of Rogers[3] and give a standard expansion formula for the functions. In virtue of this standard expansion a G^∞ function on Z is naturally extended to a wider space $\mathrm{dbl}(Z)$ called the doubling of Z.

In Sec. IV we investigate integration of functions first on the body and next on the whole complex superspace. We obtain our main theorem about the consistency of integration. We prove the consistency of integration on the space $\mathrm{dbl}(Z)$ because $\mathrm{dbl}(Z)$ admits more general variable changes than Z does and it makes the proof simple. The result on the space Z is obtained as a corollary of this general result.

Some properties of determinant of matrices over a σ-commutative algebra, which we need to calculate the Jacobian, are given in the Appendix.

Throughout the paper G is a finite Abelian group with a sign σ, that is, σ is a function of $G \times G$ to the complex field $\mathbb{C}$ satisfying

$$\sigma(\alpha+\beta,\gamma) = \sigma(\alpha,\gamma)\sigma(\beta,\gamma) \quad \text{for } \alpha,\beta,\gamma \in G,$$

and

$$\sigma(\alpha,\beta)\sigma(\beta,\alpha) = 1 \quad \text{for } \alpha,\beta \in G.$$

II. INVOLUTIONS IN σ-COMMUTATIVE ALGEBRAS

Let $A = \oplus_{\alpha\in G} A_\alpha$ be a σ-commutative G-graded algebra over $\mathbb{C}$; for any $a \in A_\alpha$ and $b \in A_\beta$, $ab = \sigma(\alpha,\beta)ba$.

A mapping $^*: A \to A$ is an *involution* of A, if it satisfies the following:

(1) $a^{**} = a$ for $a \in A$;

(2) $(a+b)^* = a^* + b^*$ for $a,b \in A$;

(3) $(ca)^* = \bar{c}a^*$ for $c \in \mathbb{C}$ and $a \in A$,

where $\bar{c}$ means the complex conjugate of c;

(4) $(ab)^* = b^*a^*$ for $a,b \in A$.

If moreover it satisfies

(5) $a^* \in A_\alpha$ for any $a \in A_\alpha$ and $\alpha \in G$,

then * is called a *conjugation* of A. On the other hand, if it satisfies

(6) $a^* \in A_{-\alpha}$ for any $a \in A_\alpha$ and $\alpha \in G$,

then * is called a *transposition* of A.

Let A and B be a σ-commutative algebras with a conjugation (resp. transposition)*. On the graded tensor product $A \otimes_{\mathbb{C}} B$ we define * by

$$(a\otimes b)^* = \sigma(\beta,\alpha)a^* \otimes b^* \quad \text{for } a \in A_\alpha,\ b \in B_\beta,\ \alpha,\beta \in G. \tag{2.1}$$

Then * is a conjugation (resp. transposition) on $A \otimes_{\mathbb{C}} B$.

Let V be a G-graded vector space over $\mathbb{C}$. A mapping $^*: V \to V$ is an involution of V, if it satisfies (1)–(3) above with A replaced by V. It is called conjugation or transposition according as it preserves or reverses the grade. Let $\mathbb{C}[V]$ be the σ-symmetric algebra of V over $\mathbb{C}$, which is, by defini-

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tion, the quotient algebra of the tensor algebra $T(V)$ of V over $\mathbb{C}$ modulo the ideal generated by the elements $vw - \sigma(\alpha,\beta)wv$ with $v\in V_\alpha$, $w\in V_\beta$, and $\alpha,\beta\in G$. An involution on V is naturally extended to the $\mathbb{C}[V]$ as follows: For $c\in\mathbb{C}$ and $v_1,\ldots,v_n\in V$, define

$$(cv_1\cdots v_n)^* = \bar{c}v_n^*\cdots v_1^*, \tag{2.2}$$

and extend * additively to $\mathbb{C}[V]$. The extended * is a conjugation (resp. transposition) of $\mathbb{C}[V]$, if so is the original *.

We decompose G into a direct sum of cyclic groups; $G = G_{(1)} \oplus \cdots \oplus G_{(n)}$, where $G_{(i)}$ is a cyclic group of order n_i. Let α_i be a generator of $G_{(i)}$. As was discussed in Ref. 4, the sign σ is given as follows on G. For integers $1\leqslant i,j\leqslant n$, let λ_{ij} be in $\mathbb{C}$ such that $\lambda_{ji} = 1/\lambda_{ij}$, $(\lambda_{ij})^{n_i} = (\lambda_{ij})^{n_j} = 1$, and λ_{ii} is 1 or -1 according as α_i is even or odd. Then for $\alpha = l_1\alpha_1 + \cdots + l_n\alpha_n$ and $\beta = m_1\alpha_1 + \cdots + m_n\alpha_n$ in G, σ is given by

$$\sigma(\alpha,\beta) = \prod_{i,j} (\lambda_{ij})^{l_i m_j}. \tag{2.3}$$

Let $G_0 = \{\alpha\in G \mid \sigma(\alpha,\alpha) = 1\}$ be the even part of G. A factor system ϕ associated with the even sign $\sigma_0 = \sigma|_{G_0\times G_0}$ of G_0 is a mapping of $G_0\times G_0$ to $\mathbb{C} - \{0\}$ satisfying

(i) $\phi(\alpha,\beta+\gamma)\phi(\beta,\gamma) = \phi(\alpha,\beta)\phi(\alpha+\beta,\gamma)$,

(ii) $\sigma(\alpha,\beta) = \phi(\alpha,\beta)/\phi(\beta,\alpha)$,

for any $\alpha,\beta,\gamma\in G_0$.

We define a mapping ψ: $G\times G\to\mathbb{C} - \{0\}$ as follows:

$$\psi(\alpha,\beta) = \prod_{i<j} (\lambda_{ij})^{l_i m_j} \tag{2.4}$$

for $\alpha = \Sigma l_i\alpha_i$ and $\beta = \Sigma m_j\alpha_j$ in G. By definition this ψ is bimultiplicative, that is,

$$\psi(\alpha+\beta,\gamma) = \psi(\alpha,\gamma)\psi(\beta,\gamma),$$

$$\psi(\alpha,\beta+\gamma) = \psi(\alpha,\beta)\psi(\alpha,\gamma),$$

for $\alpha,\beta,\gamma\in G$. So ψ satisfies

$$\psi(\alpha,\beta+\gamma)\psi(\beta,\gamma) = \psi(\alpha,\beta)\psi(\alpha+\beta,\gamma),$$

and

$$\begin{aligned}\psi(\alpha,0) = \psi(0,\alpha) &= \psi(\alpha,\beta)\psi(-\alpha,\beta)\\ &= \psi(\alpha,\beta)\psi(\alpha,-\beta) = 1.\end{aligned} \tag{2.5}$$

Moreover, by (2.3) and (2.4) we have

$$\psi(\alpha,\beta)/\psi(\beta,\alpha) = \pm\sigma(\alpha,\beta), \tag{2.6}$$

for $\alpha,\beta\in G$ and specifically $\psi(\alpha,\beta)/\psi(\beta,\alpha) = \sigma(\alpha,\beta)$ for $\alpha,\beta\in G_0$. Thus $\psi_0 = \psi|_{G_0\times G_0}$ is a factor system associated with σ_0. This factor system was defined by Scheunert.[4]

In order to simplify our calculation we need to introduce another factor system associated with σ_0. First we define a mapping t: $G\to\mathbb{C} - \{0\}$ as follows:

$$t(\alpha) = \begin{cases}\psi(\beta,\beta)^2 \text{ with } \alpha = 2\beta, & \text{if } \alpha\in 2G,\\ \sqrt{\psi(\alpha,\alpha) + i0}, & \text{if } \alpha\in G - 2G,\end{cases}$$

where $\sqrt{z+i0}$ means $\sqrt{r}e^{i\theta/2}$ for $z = re^{i\theta}$ with $-\pi < \theta\leqslant\pi$.

We claim that t is well defined. In fact, if $2\beta = 2\gamma$ for $\beta,\gamma\in G$, then

$$\begin{aligned}\psi(\beta,\beta)^2 &= \psi(2\beta,\beta) = \psi(2\gamma,\beta) = \psi(\gamma,\beta)^2\\ &= \psi(\gamma,2\beta) = \psi(\gamma,2\gamma) = \psi(\gamma,\gamma)^2.\end{aligned}$$

By the definition of t we have

$$t(0) = 1, \quad t(\alpha) = t(-\alpha), \quad t(2\alpha) = \psi(\alpha,\alpha)^2,$$

$$t(\alpha)^2 = \psi(\alpha,\alpha), \tag{2.7}$$

for $\alpha\in G$. Now we define ϕ: $G\times G\to\mathbb{C} - \{0\}$ by

$$\phi(\alpha,\beta) = [t(\alpha)t(\beta)/t(\alpha+\beta)]\psi(\alpha,\beta) \tag{2.8}$$

for $\alpha,\beta\in G$. Then $\phi_0 = \phi|_{G_0\times G_0}$ is a factor system associated with σ_0, and moreover ϕ has the following properties:

$$\begin{aligned}\phi(\alpha,0) = \phi(0,\alpha) = \phi(\alpha,\alpha) = \phi(\alpha,-\alpha)\\ = \phi(2\alpha,-\alpha) = 1,\end{aligned} \tag{2.9}$$

$$\phi(-\alpha,-\beta) = \phi(\alpha,\beta), \tag{2.10}$$

$$\phi(\alpha,\beta)\phi(\beta,\alpha) = 1, \tag{2.11}$$

$$\phi(\alpha,\beta)^2 = \phi(\alpha,\beta)/\phi(\beta,\alpha) = \pm\sigma(\alpha,\beta), \tag{2.12}$$

$$\phi(2\alpha,2\beta) = \sigma(\alpha,\beta)^2, \tag{2.13}$$

for $\alpha,\beta\in G$.

In fact, (2.9) and (2.10) follow from (2.5), (2.7), and (2.8), and (2.12) follows from (2.6), (2.8), and (2.11). Now we show (2.11) and (2.13). For $\alpha,\beta\in G$ we have

$$\begin{aligned}\phi(\alpha,\beta)\phi(\beta,\alpha) &= [t(\alpha)t(\beta)/t(\alpha+\beta)]\psi(\alpha,\beta)\\ &\quad\times[t(\beta)t(\alpha)/t(\beta+\alpha)]\psi(\beta,\alpha)\\ &= [t(\alpha)^2t(\beta)^2/t(\alpha+\beta)^2]\psi(\alpha,\beta)\psi(\beta,\alpha)\\ &= \psi(\alpha,\alpha)\psi(\beta,\beta)\psi(\alpha,\beta)\psi(\beta,\alpha)\\ &\quad\times\psi(\alpha+\beta,\alpha+\beta)^{-1}\\ &= 1.\end{aligned}$$

For $\alpha,\beta\in G$ we have

$$\begin{aligned}\phi(2\alpha,2\beta) &= [t(2\alpha)t(2\beta)/t(2\alpha+2\beta)]\psi(2\alpha,2\beta)\\ &= [\psi(\alpha,\alpha)^2\psi(\beta,\beta)^2/\psi(\alpha+\beta,\alpha+\beta)^2]\psi(\alpha,\beta)^4\\ &= [\psi(\alpha,\beta)^2/\psi(\beta,\alpha)^2] = \sigma(\alpha,\beta)^2.\end{aligned}$$

Since $|\sigma(\alpha,\beta)| = 1$ it follows from (2.12) that $|\phi(\alpha,\beta)| = 1$ for $\alpha,\beta\in G$.

Let C be the crossed product of G_0 and $\mathbb{C}$ associated with the factor system ϕ_0, that is, C is a direct sum of one-dimensional vector spaces over $\mathbb{C}$ with generators $\mathbf{u}_\alpha$, $\alpha\in G_0$ such that $\mathbf{u}_\alpha\cdot\mathbf{u}_\beta = \phi(\alpha,\beta)\mathbf{u}_{\alpha+\beta}$. Then C is a σ-commutative algebra over $\mathbb{C}$. Furthermore, by (2.9) we see that $\mathbf{u}_0$ is the identity element of C, every $\mathbf{u}_\alpha$ is invertible and

$$\mathbf{u}_\alpha^{-1} = \mathbf{u}_{-\alpha}. \tag{2.14}$$

Remark 2.1: In general, the group of even signs of G over $\mathbb{C}$ is isomorphic to the cohomology group $H^2(G,\mathbb{C} - \{0\})$, which is, by definition, the group of equivalence classes of factor systems of G. Two factor systems ϕ and ψ are equivalent if there is a mapping t: $G\to\mathbb{C} - \{0\}$ satisfying the equality (2.8). The crossed products associated with equivalent factor systems ϕ and ψ are isomorphic. It is also known that we can choose, from every equivalence class, a representative that is bimultiplicative (see Yamazaki[5]). Actually, Sheunert's factor system ψ_0 is bimultiplicative. Our factor system ϕ_0, which is equivalent to ψ_0, is not bimultiplicative but has the good property (2.13), which makes our calculations simple as will be seen below.

Next, let G_1 denote the odd part of G and let L be a G_1 set

(a linearly ordered G_1-graded set). Let V be a G_1-graded vector space with generators $\mathbf{v}_l$, $l\in L$, such that the grade of $\mathbf{v}_l$ is $g(l)$. Let B be the σ-symmetric algebra (the generalized Grassman algebra) of V over $\mathbb{C}$. The graded tensor product $A = C\otimes_{\mathbb{C}} B$ of C and B which were constructed above is a finite-dimensional σ-commutative algebra over $\mathbb{C}$. Elements of A are called (*complex*) *supernumbers*. In the subsequence of this paper this algebra A of supernumbers is fixed.

Now we shall determine all the conjugations and transpositions of C. We need the following lemma. Since $C_0 = \mathbb{C}\mathbf{u}_0$ is isomorphic to $\mathbb{C}$, $\mathbb{C}$ is considered to be a subalgebra of C and of A as well.

Lemma 2.2: Let $f(X)\in\mathbb{C}[X]$ be a nonzero separable polynomial, then all the roots of $f(X)$ in A_0 are in $\mathbb{C}$.

Proof: Since f is separable, $f(X) = (X-c_1)\times(X-c_2)\cdots(X-c_n)$, where $c_i\in\mathbb{C}$ are all different. Let $a\in A_0$ be a root of $f(X)$, that is, $(a-c_1)\times(a-c_2)\cdots(a-c_n) = 0$. The a is written as $a = a_0 + s_0$, where $a_0\in\mathbb{C}$ and s_0 is nilpotent. Since the c_i are different, the $a_0 - c_i$ are nonzero except for one index, say i_0. Then the $a - c_i$ for $i\neq i_0$ are invertible and so we get $a = c_{i_0}\in\mathbb{C}$.

Proposition 2.3: We have the following.

(i) If $\bar{}$ is a conjugation of A, then there is a homomorphism γ of G_0 to $\mathbb{C}$ (in other words γ is a character of G_0), such that

$$\overline{\mathbf{u}_\alpha} = \gamma(\alpha)\mathbf{u}_\alpha \quad \text{for } \alpha\in G_0.$$

(ii) If $*$ is a transposition of A, then there is a homomorphism γ of G_0 to $\{1,-1\}$ such that

$$\mathbf{u}^* = \gamma(\alpha)\mathbf{u}_{-\alpha} \quad \text{for } \alpha\in G_0.$$

Proof: Let $\bar{}$ be a conjugation of A. Set $\gamma(\alpha) = \mathbf{u}_{-\alpha}\,\overline{\mathbf{u}_\alpha}$. Then by (2.10) we have

$$\begin{aligned}\gamma(\alpha)\gamma(\beta) &= \mathbf{u}_{-\alpha}\,\overline{\mathbf{u}_\alpha}\mathbf{u}_{-\beta}\,\overline{\mathbf{u}_\beta} = \mathbf{u}_{-\beta}\mathbf{u}_{-\alpha}\,\overline{\mathbf{u}_\beta\mathbf{u}_\alpha}\\ &= \phi(-\beta,-\alpha)\,\mathbf{u}_{-\alpha-\beta}\,\overline{\phi(\beta,\alpha)\,\mathbf{u}_{\alpha+\beta}}\\ &= \mathbf{u}_{-\alpha-\beta}\,\overline{\mathbf{u}_{\alpha+\beta}} = \gamma(\alpha+\beta),\end{aligned}$$

for $\alpha,\beta\in G_0$. Therefore γ is a homomorphism of G_0 to A_0. Hence for any $\alpha\in G_0$ of order n, we have $\gamma(\alpha)^n = \gamma(n\alpha) = \gamma(0) = 1$, that is, $\gamma(\alpha)$ is a root of the separable polynomial $X^n - 1$. By Lemma 2.2 we see $\gamma(\alpha)\in\mathbb{C}$. It follows that γ is a character of G_0 and $\overline{\mathbf{u}_\alpha} = \gamma(\alpha)\mathbf{u}_{-\alpha}^{-1} = \gamma(\alpha)\mathbf{u}_\alpha$.

If $*$ is a transposition of A, then set $\gamma(\alpha) = \mathbf{u}_\alpha\mathbf{u}_\alpha^*$. Then in the same way as above we see γ is a character of G_0 and $\mathbf{u}_\alpha^* = \gamma(\alpha)\mathbf{u}_{-\alpha}$. Since

$$\mathbf{u}_\alpha^{**} = (\gamma(\alpha)\mathbf{u}_{-\alpha})^* = \overline{\gamma(\alpha)}\mathbf{u}_{-\alpha}^* = \overline{\gamma(\alpha)}\gamma(-\alpha)\mathbf{u}_\alpha = \mathbf{u}_\alpha,$$

we have $\gamma(\alpha)^2 = 1/\overline{\gamma(\alpha)}\gamma(-\alpha) = 1$, which implies $\gamma(\alpha) = \pm 1$.

Let $*$ be a transposition of A, then by Proposition 2.3 (ii), we see $\mathbf{u}_\alpha^* = \pm\mathbf{u}_{-\alpha}$ for any $\alpha\in G_0$. If $\mathbf{u}_\alpha^* = \mathbf{u}_{-\alpha}$ holds for every $\alpha\in G_0$, $*$ is called *standard*.

Proposition 2.4: If $*$ is a standard transposition of A, then the additive mapping $\bar{}: A\to A$ defined by

$$\bar{a} = \mathbf{u}_{2\alpha}a^* \quad \text{for } \alpha\in G \text{ and } a\in A_\alpha \tag{2.15}$$

is a conjugation of A.

Proof: First note that (2.15) makes sense, because 2α is in G_0 for any $\alpha\in G$. We have by (2.14)

$$\bar{\bar{a}} = \mathbf{u}_{2\alpha}(\mathbf{u}_{2\alpha}a^*)^* = \mathbf{u}_{2\alpha}a\mathbf{u}_{2\alpha}^* = a\mathbf{u}_{2\alpha}\mathbf{u}_{-2\alpha} = a,$$

for $a\in A_\alpha$. Moreover for $a\in A_\alpha$ and $b\in A_\beta$, by (2.13) we have

$$\begin{aligned}\overline{ab} &= \mathbf{u}_{2\alpha+2\beta}(ab)^* = \phi(2\beta,2\alpha)^{-1}\mathbf{u}_{2\beta}\mathbf{u}_{2\alpha}b^*a^*\\ &= \sigma(\alpha,\beta)^2\sigma(2\alpha,-\beta)\mathbf{u}_{2\beta}b^*\mathbf{u}_{2\alpha}a^* = \bar{b}\,\bar{a}.\end{aligned}$$

Thus $\bar{}$ is a conjugation of A.

The conjugation $\bar{}$ in Proposition 2.4 is said to be associated with the standard transposition $*$ of A.

Now we define a transposition $*$ of A as follows. For $c\in\mathbb{C}$ and $\alpha\in G_0$ define

$$(c\mathbf{u}_\alpha)^* = \bar{c}\mathbf{u}_{-\alpha},$$

and extend $*$ additively to C. Then, $*$ is a transposition of C, as is readily seen from (2.14). To define a transposition of B, suppose the G_1 set L used to define B has a transposition $*$, that is, $*$ is a mapping from L to L such that $g(l^*) = -g(l)$ and $l^{**} = l$ for all $l\in L$. Then the G-graded vector space V defined by L has a transposition $*$ induced from the transposition $*$ of L; $(c\mathbf{v}_l)^* = \bar{c}\mathbf{v}_{l^*}$ for $c\in\mathbb{C}$ and $l\in L$. Now the σ-symmetric algebra B of V over $\mathbb{C}$ has the transposition $*$ given by (2.2) and $A = C\otimes B$ also has the transposition $*$ given as (2.1). Let $\bar{}$ be the conjugation of A associated with $*$. Then by (2.9) we have

$$\overline{\mathbf{u}_\alpha} = \mathbf{u}_\alpha \quad \text{for } \alpha\in G_0,$$

and

$$\overline{\mathbf{v}_M} = \mathbf{u}_{2g(M)}\otimes\mathbf{v}_{M^*},$$

where $M = \{l_1,\ldots,l_m\}\subset L$, $\mathbf{v}_M = \mathbf{v}_{l_1}\cdots\mathbf{v}_{l_m}$, $g(M) = g(l_1) + \cdots + g(l_m)$, and $\mathbf{v}_{M^*} = \mathbf{v}_{l_m^*}\cdots\mathbf{v}_{l_1^*}$. In this paper the transposition $*$ and the associated conjugation $\bar{}$ play important roles.

III. COMPLEX SUPERSPACE AND DIFFERENTIABLE FUNCTIONS

As we stated in Sec. II, A is the algebra of complex supernumbers with the transposition $*$ and its associated conjugation $\bar{}$. Also A is a Banach algebra with a suitable norm (see Ref. 1). In our previous paper[1] we developed differential caluculus over the real superspace. In this section we study differentiable functions defined on superspace parametrized in A. To accomplish this we first decompose A into the real and the imaginary parts.

For $\alpha\in G$ we define the real part $\mathrm{Re}(A_\alpha)$ and the imaginary part $\mathrm{Im}(A_\alpha)$ of A_α by

$$\mathrm{Re}(A_\alpha) = \{a\in A_\alpha \mid \bar{a} = a\},\quad \mathrm{Im}(A_\alpha) = \{a\in A_\alpha \mid \bar{a} = -a\}.$$

Then we have

$$A_\alpha = \mathrm{Re}(A_\alpha)\oplus\mathrm{Im}(A_\alpha) \quad \text{and} \quad \mathrm{Im}(A_\alpha) = \mathbf{i}\,\mathrm{Re}(A_\alpha),$$

where $\mathbf{i} = \sqrt{-1}$. Thus an element $c\in A_\alpha$ is written as

$$c = \mathrm{Re}(c) + \mathrm{Im}(c) = a + \mathbf{i}b \quad \text{with } a,b\in\mathrm{Re}(A_\alpha). \tag{3.1}$$

Let $I = \{1,\ldots,p,p+1,\ldots,p+q\}$ be a G set such that $g(i)$ are even for $i = 1,\ldots,p$ and odd for $i = p+1,\ldots,p+q$. The direct sum $Z = \oplus_{i\in I} A_{g(i)}$ is called the (*generalized*) *complex superspace* over A. Here Z is decomposed as follows:

$$Z = \bigoplus_{i\in I}(\mathrm{Re}(A_{g(i)}) \oplus \mathrm{Im}(A_{g(i)}))$$
$$= \Big(\bigoplus_{i\in I}\mathrm{Re}(A_{g(i)})\Big) \oplus \Big(\bigoplus_{i\in I}\mathrm{Im}(A_{g(i)})\Big).$$

Let U be a domain of Z and let A^U denote the set of A-valued functions defined on U. A function $f\in A^U$ is *right differentiable* at $z_0\in U$, if there are constants a_i, $b_i\in A$ such that

$$f(z_0+z) - f(z_0) = \sum_{i\in I}(a_i \mathrm{Re}(z^i) + b_i\, \mathrm{Im}(z^i)) + o(\|z\|)$$

as $z = (z^1,\ldots,z^{p+q})\in Z$ approaches 0. The constants a_i and b_i are called the *right differential coefficients* of f at z_0. In virtue of (3.1) we always write

$$z^i = x^i + \mathbf{i}y^i \quad \text{with } x^i,y^i\in\mathrm{Re}(A_{g(i)}), \tag{3.2}$$

and the coefficients a_i and b_i are written as $\partial f(\partial x^i)^{-1}$ and $-\mathbf{i}\,\partial f(\partial y^i)^{-1}$, respectively.

Using the relations (3.2) and $\bar{z}^i = \overline{x^i + \mathbf{i}y^i} = x^i - \mathbf{i}y^i$, it is readily seen that $f\in A^U$ is right differentiable at z_0, if and only if there are constants α_i,β_i such that

$$f(z_0+z) - f(z_0) = \sum_{i\in I}(\alpha_i z^i + \beta_i \bar{z}^i) + o(\|z\|),$$

as $z\to 0$. We write $\alpha_i = \partial f(\partial z^i)^{-1}$ and $\beta_i = \partial f(\partial \bar{z}^i)^{-1}$. Then the following relations hold:

$$\begin{aligned}
&\partial f(\partial x^i)^{-1} = \partial f(\partial z^i)^{-1} + \partial f(\partial \bar{z}^i)^{-1},\\
&\partial f(\partial y^i)^{-1} = \mathbf{i}(\partial f(\partial z^i)^{-1} - \partial f(\partial \bar{z}^i)^{-1}),\\
&\partial f(\partial z^i)^{-1} = \tfrac{1}{2}(\partial f(\partial x^i)^{-1} - \mathbf{i}\,\partial f(\partial y^i)^{-1}),\\
&\partial f(\partial \bar{z}^i)^{-1} = \tfrac{1}{2}(\partial f(\partial x^i)^{-1} + \mathbf{i}\,\partial f(\partial y^i)^{-1}).
\end{aligned} \tag{3.3}$$

Remark 3.1: For an odd index i the differential coefficients are not uniquely determined, though they are unique mod $\mathrm{Ann}(A_{g(i)}) = \{a\in A \mid aA_{g(i)} = 0\}$. Therefore the equalities in (3.3) hold only mod $\mathrm{Ann}(A_{g(i)})$. However, if f is sufficiently smooth, we can choose canonical ones using the standard expansion of f stated later (Proposition 3.5), and if we understand that $\partial f(\partial x^i)^{-1}$, etc., are those canonical ones, the equalities hold exactly.

If there are continuous functions $g_i,h_i\in A^U$ such that $g_i(z) = \partial f(\partial x_i)^{-1}(z)$ and $h_i(z) = \partial f(\partial y_i)^{-1}(z)$ for $z\in U$, we say f is a G^1 function on U or $f\in G^1(U)$. We can also define $G^r(U)$, the set of r-times continuously differentiable functions and $G^\infty(U)$, the set of infinitely differentiable functions on U (see Ref. 1).

From the definition we readily have the following.

Proposition 3.2 (Chain Rule): Let K be another G set and $w = (w^k \mid k\in K)$: $U\to V\subset W = A_K$ be a G^1 mapping, where $w^k\in G^1(U)$ such that $w^k(z)\in A_{g(k)}$. Then for $f\in G^1(V)$, the composition $f(w(z))$ of f and w belongs to $G^1(U)$ and the equalities

$$\begin{aligned}
\partial f(\partial x^i)^{-1} = \sum_k (&\partial f(\partial u^k)^{-1}\,\partial u^k(\partial x^i)^{-1}\\
&+ \partial f(\partial v^k)^{-1}\,\partial v^k(\partial x^i)^{-1}),\\
\partial f(\partial y^i)^{-1} = \sum_k (&\partial f(\partial u^k)^{-1}\,\partial u^k(\partial y^i)^{-1}\\
&+ \partial f(\partial v^k)^{-1}\,\partial v^k(\partial y^i)^{-1}),
\end{aligned}$$

hold on U mod $\mathrm{Ann}(A_{g(i)})$, where $w^i = u^i + \mathbf{i}v^i$.

An element a of A is expressed as

$$a = \sum_{\alpha,M} a_{\alpha,M}\mathbf{u}_\alpha \otimes \mathbf{v}_M, \quad \alpha\in G_0, \quad M\subset L. \tag{3.4}$$

For $a\in A$ given as (3.4), its body $b(a)$ and soul $s(a)$ are defined by

$$b(a) = \sum_{\alpha\in G_0} a_{\alpha,\varnothing}\mathbf{u}_\alpha \otimes 1, \quad s(a) = \sum_{\alpha\in G_0,\, M\neq\varnothing} a_{\alpha,M}\mathbf{u}_\alpha \otimes \mathbf{v}_M.$$

Note that a is invertible if it has nonzero homogeneous body, while the soul of a is nilpotent. Moreover, for a domain U we define $b(U) = \{b(z) = (b(z^1),\ldots,b(z^{p+q}))\mid z\in U\}$ and $s(U) = \{s(z) = (s(z^1),\ldots,s(z^{p+q}))\mid z\in U\}$.

For a subset A' of A define $\mathrm{Sav}(A') = \Sigma_M\, C\otimes \mathbf{v}_M$, where M ranges over all subsets in L such that $\mathbf{v}_M A'\neq 0$. Then we have $A = \mathrm{Ann}(A')\oplus \mathrm{Sav}(A')$.

Proposition 3.3 (Taylor's expansion): Let U be a domain of Z and let $w = (w^i)$ be in the soul $s(Z)$ of Z. Let $f\in G^\infty(U)$ and suppose $z+\theta w\in U$ for all θ with $0\leqslant\theta\leqslant 1$, then

$$\begin{aligned}
&f(z+w)\\
&= \sum_{m,n=0}^{\infty}\frac{1}{m!n!}\sum f_{x^{i_m}\cdots x^{i_1}y^{k_n}\cdots y^{k_1}}(z)v^{k_1}\cdots v^{k_n}u^{i_1}\cdots u^{i_m},\\
&= \sum_{m,n=0}^{\infty}\frac{1}{m!n!}\sum f_{z^{i_m}\cdots z^{i_1}\bar{z}^{k_n}\cdots\bar{z}^{k_1}}(z)\bar{w}^{k_1}\cdots\bar{w}^{k_n}w^{i_1}\cdots w^{i_m},
\end{aligned} \tag{3.5}$$

where $z = x+\mathbf{i}y$, $w = u+\mathbf{i}v$, $f_{x^{i_m}\cdots x^{i_1}y^{k_n}\cdots y^{k_1}}$ (resp. $f_{z^{i_m}\cdots z^{i_1}\bar{z}^{k_n}\cdots\bar{z}^{k_1}}$) is the $m+n$ times derivative of f with respect to $x^{i_m},\ldots,x^{i_1},y^{k_n},\ldots,y^{k_1}$ (resp. $z^{i_m},\ldots,z^{i_1},\bar{z}^{k_n},\ldots,\bar{z}^{k_1}$) and $(i_1,\ldots,i_m)$ [resp. $(k_1,\ldots,k_n)$] ranges over I^m (resp. I^n).

Note that only a finite number of the summands in (3.5) are nonzero because the w^i are nilpotent.

Some formulas are more convenient if they are expressed in z^i and $z^{i*} = (z^i)^* = \mathbf{u}_{-2g(i)}\bar{z}^i$ instead of in z^i and $\bar{z}^i$ [recall (2.15)]. We define $\partial f(\partial z^{i*})^{-1}$ to be the constants β_i satisfying

$$f(z_0+z) - f(z_0) = \sum_{i\in I}(\alpha_i z^i + \beta_i z^{i*}) + o(\|z\|)$$

as $z\to 0$, here $\alpha_i = \partial f(\partial z^i)^{-1}$. Then we have

$$\partial f(\partial z^{i*})^{-1} = \partial f(\partial \bar{z}^i)^{-1}\mathbf{u}_{2g(i)} \tag{3.6}$$

and the Taylor expansion (3.5) of f is rewritten as

$$\begin{aligned}
f(z+w) = \sum_{m,n=0}^{\infty}\frac{1}{m!n!}&\sum f_{z^{i_m}\cdots z^{i_1}z^{k_n*}\cdots z^{k_1*}}(z)\\
&\times w^{j_1*}\cdots w^{j_n*}w^{i_1}\cdots w^{i_m}.
\end{aligned} \tag{3.7}$$

For later use we prepare the following proposition.

Proposition 3.4: Let f be homogeneous of grade $\alpha\in G$. Then we have

$$\partial f^*(\partial z^{i*})^{-1} = \sigma(g(i),\alpha - g(i))(\partial f(\partial z^i)^{-1})^*.$$

Proof: From the definition of differentiation

$(\partial f(\partial z^j)^{-1})^*$ is equal to the left derivative $((\partial z^{i^*})^{-1})f^*\partial$, which is equal to $\sigma(-\alpha+g(i),g(i))\partial f^*(\partial z^{i^*})^{-1}$. Hence the desired equality holds.

To distinguish even and odd variables, we introduce new symbols ζ^j for the odd variables z^j $(j=p+1,...,p+q)$. Let U be a saturated domain in Z, that is, $U=\bar{U}=U+s(Z)$ and f be in $G^\infty(U)$. By Taylor's theorem we have

$$f(z,\zeta)=\sum_{m,n,s,t=0}^{\infty}\frac{1}{m!n!s!t!}\sum f_{(i_m\cdots i_1;j_n^*\cdots j_1^*:k_s\cdots k_1;l_t^*\cdots l_1^*)}(b(z))s(\overset{*}{z}{}^{l_1})\cdots s(\overset{*}{z}{}^{l_t})s(z^{k_1})\cdots s(z^{k_s})\overset{*}{\zeta}{}^{j_1}\cdots\overset{*}{\zeta}{}^{j_n}\zeta^{i_1}\cdots\zeta^{i_m}$$

$$=\sum_{m,n,s,t=0}^{\infty}\frac{1}{m!n!s!t!}\sum P\left(f_{(i_m\cdots i_1;j_n^*\cdots j_1^*:k_s\cdots k_1;l_t^*\cdots l_1^*)}(b(z))\right)s(\overset{*}{z}{}^{l_1})\cdots s(\overset{*}{z}{}^{l_t})s(z^{k_1})\cdots s(z^{k_s})\overset{*}{\zeta}{}^{j_1}\cdots\overset{*}{\zeta}{}^{j_n}\zeta^{i_1}\cdots\zeta^{i_m},\qquad(3.8)$$

where

$$P\left(f_{(i_m\cdots i_1;j_n^*\cdots j_1^*:k_s\cdots k_1;l_t^*\cdots l_1^*)}(b(z))\right)$$

is the projection of

$$f_{(i_m\cdots i_1;j_n^*\cdots j_1^*:k_s\cdots k_1;l_t^*\cdots l_1^*)}(b(z))$$

to $\mathrm{Sav}(A')$, where

$$A'=A_{g(i_m)}\cdots A_{g(i_1)}A_{g(j_n)}\cdots A_{g(j_1)}s(A_{g(k_s)})\cdots s(A_{g(k_1)})s(A_{g(l_t)})\cdots s(A_{g(l_1)}).$$

If we set

$$f_{i_m\cdots i_1;j_n^*\cdots j_1^*}(z)=\sum_{s,t=0}^{\infty}\frac{1}{m!n!s!t!}\sum P\left(f_{(i_m\cdots i_1;j_n^*\cdots j_1^*:k_s\cdots k_1;l_t^*\cdots l_1^*)}(b(z))\right)\times s(\overset{*}{z}{}^{l_1})\cdots s(\overset{*}{z}{}^{l_t})s(z^{k_1})\cdots s(z^{k_s}),$$

we have

$$f(z,\zeta)=\sum f_{i_m\cdots i_1;j_n^*\cdots j_1^*}(z)\times\overset{*}{\zeta}{}^{j_1}\cdots\overset{*}{\zeta}{}^{j_n}\zeta^{i_1}\cdots\zeta^{i_m}.$$

For a G set $I=\{i_1,...,i_n\}$ with $i_1<\cdots<i_n$, we define a G set $I^*=\{i_n^*,...,i_1^*\}$ in which the grade of i_j^* is $-g(i_j)$ and $i_n^*<...<i_1^*$. There is a natural mapping $*: I\to I^*$ given by $(i_j)^*=i_j^*$. For a subset M of I, M^* is the image of M under the mapping $*$.

For $M=\{i_1<\cdots<i_m\}\subset I_1$, $\zeta^{i_1}\cdots\zeta^{i_m}$ is abbreviated as ζ^M. Now we get the following proposition.

Proposition 3.5 (Standard expansion): Let U be a saturated domain of Z and $f\in G^\infty(U)$. Then f can be uniquely expressed as follows:

$$f(z,\zeta)=\sum f_{M;N^*}(z)(\zeta^N)^*\zeta^M,\quad(z,\zeta)\in U,\qquad(3.9)$$

where M and N range over all subsets of I_1, and

(i) $f_{M;N^*}(z)$ is a G^∞ function on U_0,

(ii) $f_{M;N^*}(z)$ belongs to $\mathrm{Sav}\left(\prod_{i\in M}A_{g(i)}\cdot\prod_{j\in N^*}A_{g(j)}\right)$

for all $z\in b(U)$.

The expression (3.9) in Proposition 3.5 is called the *standard expansion* of f. The function $f_{I_1;I_1^*}$ appearing in (3.9) is called the *top* of f. The canonical derivative $\partial f(\partial\zeta^i)^{-1}$ of f with respect to ζ^i with $i\in I_1\cup I_1^*$ is defined by

$$\partial f(\partial\zeta^i)^{-1}=\epsilon_{M;N^*}\sum f_{M;N^*}(z)(\zeta^{N'})^*\zeta^{M'},$$

where $M'=M-\{i\}$, $N'^*=N^*-\{i\}$, and $(\zeta^N)^*\zeta^M=\epsilon_{M;N^*}(\zeta^{N'})^*\zeta^{M'}\zeta^i$.

The G^∞ function f is called *analytic* if $\partial f(\partial\bar{z}^i)^{-1}=0$, or equivalently, $\partial f(\partial z^{i^*})^{-1}=0$ for any $i\in I_0$. Then, f is analytic if and only if $f_{M;N^*}(z)$ is analytic for any $M,N\subset I_1$ in (3.9).

Remark 3.6: A G^1 function f satisfying $\partial f(\partial\bar{z})^{-1}=0$ is not necessarily analytic. Let A be the usual Grassmann algebra generated by two odd elements v and w over $\mathbb{C}$. Define a function f in one odd variable ξ as follows: For $\xi=av+bw\in A_1$ with $a,b\in\mathbb{C}$, $f(\xi)=abvw$. Then for $\xi_0=a_0v+b_0w\in A_1$, we have

$$f(\xi_0+\xi)-f(\xi_0)=(a_0+a)(b_0+b)vw-a_0b_0vw=(a_0b+ab_0)vw+o(\xi)=(a_0v-b_0w)\xi+o(\xi).$$

This implies $\partial f(\partial\xi)^{-1}=av-bw$ and $\partial f(\partial\bar{\xi})^{-1}=0$. However, $\partial f(\partial\xi)^{-1}$ is not differentiable, and hence f is not G^2.

Let $Z^*=A_{I^*}$ be the superspace indexed by I^*, which we call the *dual superspace* of Z. There is a natural mapping $*: Z\to Z^*$ given by $\overset{*}{z}=(\overset{*}{z}{}^{p+q},...,\overset{*}{z}{}^1)$. For a domain U of Z, the image U^* of U is a domain in Z^*.

Definition 3.7: The subset $U\times_b U^*=\{(z,z^*)|z=(z^i)\in U,\ z^*=(z^{i^*})\in U^*$ and $b(\overset{*}{z}{}^i)=b(z^{i^*}),\ i=1,...,p+q\}$ of $U\times U^*$ is called the *doubling* of U and denoted by $\mathrm{dbl}(U)$. Here U is embedded in $\mathrm{dbl}(U)$ by the mapping ι which sends z to $(z,\overset{*}{z})$. A function $f(z,z^*)$ defined on $\mathrm{dbl}(U)$ is right differentiable at (z_0,z_0^*), if there are constants $\alpha_i,\beta_i\in A$ such that

$$f(z_0+z,z_0^*+z^*)-f(z_0,z_0^*)=\sum_{i\in I}(\alpha_iz^i+\beta_iz^{i^*})+o(\|z\|+\|z^*\|)$$

as $(z,z^*)\to 0$, for $(z,z^*)\in\mathrm{dbl}(Z)$ with $(z_0+z,\ z_0^*+z^*)\in\mathrm{dbl}(U)$. We write $\alpha_i=\partial f(\partial z^i)^{-1}$ and $\beta_i=\partial f(\partial z^{i^*})^{-1}$.

Some formulas discussed above hold also for functions on the doubling of Z and we list them below.

Proposition 3.8 (Chain Rule): Let U' be a domain of $\mathrm{dbl}(Z)$. Let K be another G set and $(w,w^*)=(w^k|k\in K\cup K^*)$: $U'\to V'\subset\mathrm{dbl}(W)=A_K\times_bA_{K^*}$ be a G^1 map-

ping, where w^k and w^{k*} are G^1 functions on U' such that $w^k(z,z^*)\in A_{g(k)}$, $w^{k*}(z,z^*)\in A_{-g(k)}$, and $b(w^k(z,z^*))^* = b(w^{k*}(z,z^*))$. Then for $f\in G^1(V')$, the composition $f(w(z,z^*),w^*(z,z^*))$ of f and (w,w^*) belongs to $G^1(U')$ and we have

$$\partial f(\partial z^i)^{-1} = \sum_k (\partial f(\partial w^k)^{-1}\partial w^k(\partial z^i)^{-1} + \partial f(\partial w^{k*})^{-1}\partial w^{k*}(\partial z^i)^{-1})$$

mod $\mathrm{Ann}(A_{g(i)})$ and

$$\partial f(\partial z^{i*})^{-1} = \sum_k (\partial f(\partial w^k)^{-1}\partial w^k(\partial z^{i*})^{-1} + \partial f(\partial w^{k*})^{-1}\partial w^{k*}(\partial z^{i*})^{-1})$$

mod $\mathrm{Ann}(A_{-g(i)})$.

Proposition 3.9 (Taylor's expansion): Let (w,w^*) be in the soul $s(Z\times_b Z^*) = s(Z)\times s(Z^*)$ of $\mathrm{dbl}(Z)$. Suppose $(z+\theta w, z^*+\theta w^*)$ is in U', a domain in $\mathrm{dbl}(Z)$, for all θ with $0\leqslant\theta\leqslant 1$. Then for a G^∞ function on U' we have

$$f(z+w,z^*+w^*) = \sum_{m,n=0}^{\infty}\frac{1}{m!n!}\sum f_{z^{i_m}\cdots z^{i_1}z^{j_n^*}\cdots z^{j_1^*}}(z,z^*)\times w^{j_1^*}\cdots w^{j_n^*}w^{i_1}\cdots w^{i_m}.$$

Proposition 3.10: Any G^∞ function $f(z)$ on a domain U of Z is uniquely extended to a G^∞ function on $\mathrm{dbl}(U)$. Conversely, the restriction of a G^∞ function on $\mathrm{dbl}(U)$ to U is a G^∞ function on U. Therefore we have

$$G^\infty(U)\cong G^\infty(\mathrm{dbl}(U)).$$

Proof: Since any G^∞ function on U can be expressed as (3.8), it is extended to $\mathrm{dbl}(U)$.

Proposition 3.11 (Standard expansion): Let U be a saturated domain of Z and $f\in G^\infty(\mathrm{dbl}(U))$. Then f can be uniquely expressed as follows:

$$f(z,z^*,\zeta,\zeta^*) = \sum f_{M;N^*}(z,z^*)\zeta^{N^*}\zeta^M,\quad (z,z^*,\zeta,\zeta^*)\in\mathrm{dbl}(U), \tag{3.10}$$

where M and N range over all subsets of I_1, and

(i) $f_{M;N^*}(z,z^*)$ is a G^∞ function on $\mathrm{dbl}(U)_0 = \mathrm{dbl}(U_0)$,

(ii) $f_{M;N^*}(z,z^*)$ belongs to $\mathrm{Sav}\left(\prod_{i\in M}A_{g(i)}\cdot\prod_{j\in N^*}A_{g(j)}\right)$ for all $(z,z^*)\in b(\mathrm{dbl}(U)) = \{(z,\bar z)\,|\,z\in b(U)\}\cong b(U)$.

The expression (3.10) in Proposition 3.5 is called the *standard expansion* of f. The function $f_{I_1;I_1^*}$ appearing in (3.10) is called the *top* of f.

Remark 3.12: If $f(z)\in G^\infty(U)$ is an entire function of x and y, that is, it has a Taylor expansion with infinite radius of convergence, then it is extended to a G^∞ function on $Z\times Z^*$.

IV. INTEGRATION AND CONSISTENCY THEOREM

Before we define integration on a general superspace, we introduce integration on the body.

Let Z be the superspace given in the preceding section. With a point $z=(z^1,\ldots,z^p,0,\ldots,0)$ of the body $b(Z)$ of Z we associate the point $\tilde z=(\tilde z^1,\ldots,\tilde z^p)$ of the complex p-dimensional space $\mathbb{C}^p$ such that $z^i=\tilde z^i\mathbf{u}_{g(i)}$, $\tilde z^i\in\mathbb{C}$. Let V be a domain in the body $b(Z)$. Then $\tilde V=\{\tilde z\,|\,z\in V\}$ is a domain of $\mathbb{C}^p$. Let f be an A-valued function defined on V. Then f is written uniquely as

$$f(z)=\sum_{\alpha,M}f_{\alpha,M}(z)\mathbf{u}_\alpha\otimes\mathbf{v}_M,\quad z\in V,$$

where $\alpha\in G_0$, $M\subset L$, and $f_{\alpha,M}(z)\in\mathbb{C}$. The functions $\tilde f_{\alpha,M}$ which are defined by

$$\tilde f_{\alpha,M}(\tilde z)=f_{\alpha,M}(z),\quad z\in V,$$

are $\mathbb{C}$-valued functions on the domain $\tilde V$.

Definition 4.1: Let $f\in A^V$ be an integrable function, that is, all the $\tilde f_{\alpha,M}$ are integrable on $\tilde V$. We define

$$\int_V f(z)dz\,dz^* = (-2\mathrm{i})^p\sum_{\alpha,M}\int_{\tilde V}\tilde f_{\alpha,M}(\tilde x,\tilde y)d\tilde x\,d\tilde y\,\mathbf{u}_\alpha\otimes\mathbf{v}_M,$$

where $\tilde z^i=\tilde x^i+\mathrm{i}\tilde y^i$.

Definition 4.2: Let J be a G set and $w=(w^j)$ be a C^1 mapping from V to A_J. For convenience, $J\cup J$ denotes the G set defined by the disjoint union of J and its copy. The $(J\cup J)\times(I\cup I)$ matrices

$$D\begin{pmatrix}(u,v)\\(x,y)\end{pmatrix}=\begin{pmatrix}D(u/x) & D(u/y)\\ D(v/x) & D(v/y)\end{pmatrix} = \begin{pmatrix}(\partial u^j(\partial x^i)^{-1}) & (\partial u^j(\partial y^i)^{-1})\\ (\partial v^j(\partial x^i)^{-1}) & (\partial v^j(\partial y^i)^{-1})\end{pmatrix},$$

$$D\begin{pmatrix}(w,\bar w)\\(z,\bar z)\end{pmatrix}=\begin{pmatrix}D(w/z) & D(w/\bar z)\\ D(\bar w/z) & D(\bar w/\bar z)\end{pmatrix} = \begin{pmatrix}(\partial w^j(\partial z^i)^{-1}) & (\partial w^j(\partial\bar z^i)^{-1})\\ (\partial\bar w^j(\partial z^i)^{-1}) & (\partial\bar w^j(\partial\bar z^i)^{-1})\end{pmatrix},$$

and the $(J\cup J^*)\times(I\cup I^*)$ matrix

$$D\begin{pmatrix}(w,w^*)\\(z,z^*)\end{pmatrix}=\begin{pmatrix}D(w/z) & D(w/z^*)\\ D(w^*/z) & D(w^*/z^*)\end{pmatrix} = \begin{pmatrix}(\partial w^j(\partial z^i)^{-1}) & (\partial w^j(\partial\bar z^{i*})^{-1})\\ (\partial\overset{*}{w}{}^j(\partial z^i)^{-1}) & (\partial\overset{*}{w}{}^j(\partial\bar z^{i*})^{-1})\end{pmatrix}$$

are called the Jacobian matrices for w. If J is even and $|I|=|J|$, the determinants of $D((u,v)/(x,y))$, $D((w,\bar w)/(z,\bar z))$, and $D((w,w^*)/(z,z^*))$ are called the Jacobians for w, and are denoted by $\Delta((u,v)/(x,y))$, $\Delta((w,\bar w)/(z,\bar z))$, and $\Delta((w,w^*)/(z,z^*))$, respectively.

For a while I and J will be even G sets such that $|I|=|J|$.

Proposition 4.3: Under the situation in Definition 4.2 we have $\Delta((w,\bar w)/(z,\bar z))=\Delta((u,v)/(x,y))$.

Proof: By (3.3) we get

$$D\begin{pmatrix}(w,\bar w)\\(z,\bar z)\end{pmatrix}=\frac{1}{2}\begin{pmatrix}D\left(\frac{u}{x}\right)-\mathrm{i}D\left(\frac{u}{y}\right)+\mathrm{i}D\left(\frac{v}{x}\right)+D\left(\frac{v}{y}\right) & D\left(\frac{u}{x}\right)+\mathrm{i}D\left(\frac{u}{y}\right)+\mathrm{i}D\left(\frac{v}{x}\right)-D\left(\frac{v}{y}\right)\\ D\left(\frac{u}{x}\right)-\mathrm{i}D\left(\frac{u}{y}\right)-\mathrm{i}D\left(\frac{v}{x}\right)-D\left(\frac{v}{y}\right) & D\left(\frac{u}{x}\right)+\mathrm{i}D\left(\frac{u}{y}\right)-\mathrm{i}D\left(\frac{v}{x}\right)+D\left(\frac{v}{y}\right)\end{pmatrix}.$$

Applying the elementary transformations (see the Appendix, Proposition A.1), we can calculate as follows:

$$\Delta\left(\frac{(w,\bar{w})}{(z,\bar{z})}\right)=\left(\frac{1}{2}\right)^{2p}\det\begin{pmatrix}2D\left(\frac{u}{x}\right)-2iD\left(\frac{u}{y}\right) & 2D\left(\frac{u}{x}\right)+2iD\left(\frac{u}{y}\right)\\ -iD\left(\frac{v}{x}\right)-D\left(\frac{v}{y}\right) & -iD\left(\frac{v}{x}\right)+D\left(\frac{v}{y}\right)\end{pmatrix}$$

$$=\left(\frac{1}{2}\right)^{p}\det\begin{pmatrix}2D(u/x) & iD(u/y)\\ -2iD(v/x) & D(v/y)\end{pmatrix}=\Delta\left(\frac{(u,v)}{(x,y)}\right).$$

Let

$$D\left(\frac{(\tilde{u},\tilde{v})}{(\tilde{x},\tilde{y})}\right)=\begin{pmatrix}D(\tilde{u}/\tilde{x}) & D(\tilde{u}/\tilde{y})\\ D(\tilde{v}/\tilde{x}) & D(\tilde{v}/\tilde{y})\end{pmatrix},$$

where $D(\tilde{u}/\tilde{x})$, etc., are the ordinary Jacobian matrices.

Proposition 4.4: Under the above situation we have

$$D\{(u,v)/(x,y)\}=U_{J\cup J}D\{(\tilde{u},\tilde{v})/(\tilde{x},\tilde{y})\}U_{I\cup I}^{-1},$$

where

$$U_{J\cup J}=\begin{pmatrix}U_J & 0\\ 0 & U_J\end{pmatrix}$$

and U_J is a $J\times\tilde{J}$ matrix given by $(U_J)^j_k=\delta^j_k\mathbf{u}_{g(j)}$ ($\tilde{J}$ is the G set obtained from J by redefining the grade of every element of J to be 0). Moreover, we have

$$\Delta\{(u,v)/(x,y)\}=(\det U_J)^2\Delta\{(\tilde{u},\tilde{v})/(\tilde{x},\tilde{y})\}(\det U_I)^{-2},$$

and, in particular, if $I=J$, then we have

$$\Delta\{(u,v)/(x,y)\}=\Delta\{(\tilde{u},\tilde{v})/(\tilde{x},\tilde{y})\}.$$

Proof: Since $u^j(z)=\tilde{u}^j(\tilde{z})\mathbf{u}_{g(j)}$ and $z^i=\tilde{z}^i\mathbf{u}_{g(i)}$ we get

$$\partial u^j(\partial x^i)^{-1}=\frac{\partial\tilde{u}^j}{\partial\tilde{x}^i}\mathbf{u}_{g(j)}\mathbf{u}_{g(i)}^{-1}$$

by the definition of differentiation. This implies $D(u/x)=U_JD(\tilde{u}/\tilde{x})U_I^{-1}$ and thus we obtain the first equality. By the multiplicative property of determinant we get the other equalities.

Proposition 4.5: Under the above situation we have

$$\Delta\{(w,w^*)/(z,z^*)\}=\Delta\{(\tilde{u},\tilde{v})/(\tilde{x},\tilde{y})\}.$$

Therefore $\Delta\{(w,w^*)/(z,z^*)\}$ is a real number.

Proof: Note that $U_IU_I^T$ is an $I\times I$ matrix of which (i,k) element is $\delta^i_k\mathbf{u}_{2g(i)}$. By (3.6) we have

$$D\left(\frac{(w,w^*)}{(z,z^*)}\right)=\begin{pmatrix}D(w/z) & D(w/\bar{z})U_IU_I^T\\ (U_JU_J^T)^{-1}D(\bar{w}/z) & (U_JU_J^T)^{-1}D(\bar{w}/\bar{z})U_IU_I^T\end{pmatrix}$$

$$=\begin{pmatrix}1 & 0\\ 0 & (U_JU_J^T)^{-1}\end{pmatrix}D\left(\frac{(w,\bar{w})}{(z,\bar{z})}\right)\begin{pmatrix}1 & 0\\ 0 & U_IU_I^T\end{pmatrix}.$$

Therefore we get

$$\Delta\{(w,w^*)/(z,z^*)\}=\det(U_JU_J^T)^{-1}\Delta\{(w,\bar{w})/(z,\bar{z})\}\det(U_IU_I^T)$$

$$=(\det U_J)^{-2}\Delta\{(w,\bar{w})/(z,\bar{z})\}(\det U_I)^2,$$

because $\det U_I^T=\sigma(g(I),g(\tilde{I})-g(I))\det U_I=\det U_I$ by Proposition A.2 in the Appendix. By Propositions 4.3 and 4.4, the last term is equal to

$$(\det U_J)^{-2}\Delta\{(u,v)/(x,y)\}(\det U_I)^2$$

$$=\Delta\{(\tilde{u},\tilde{v})/(\tilde{x},\tilde{y})\}.$$

Proposition 4.6: Let I and J be even G sets with $|I|=|J|$ and $Z=A_I$ and $W=A_J$. Let U and V be domains in $b(Z)$ and $b(W)$, respectively. Let $w=(w^i)=(u^i+iv^i)$ be a one to one C^1 mapping from U onto V such that $\Delta\{(w,w^*)/(z,z^*)\}$ is nonzero. Then for an integrable function f on V we have

$$\int_U f(w(z))\left|\Delta\left(\frac{(w,w^*)}{(z,z^*)}\right)\right|dz\,dz^*=\int_V f(w)dw\,dw^*.$$

Proof: By Definition 4.1 and Proposition 4.5 we have

$$\int_U f(w(z))\left|\Delta\left(\frac{(w,w^*)}{(z,z^*)}\right)\right|dz\,dz^*$$

$$=(-2i)^p\sum_{\alpha,M}\int_{\tilde{U}}\tilde{f}_{\alpha,M}(\tilde{u}(\tilde{x},\tilde{y}),\tilde{v}(\tilde{x},\tilde{y}))$$

$$\times\left|\Delta\left(\frac{(\tilde{u},\tilde{v})}{(\tilde{x},\tilde{y})}\right)\right|d\tilde{x}\,d\tilde{y}\,\mathbf{u}_\alpha\otimes\mathbf{v}_M.$$

By the usual formula of change of coordinates, the last is equal to

$$(-2i)^p\sum_{\alpha,M}\int_{\tilde{V}}\tilde{f}_{\alpha,M}(\tilde{u},\tilde{v})d\tilde{u}\,d\tilde{v}\,\mathbf{u}_\alpha\otimes\mathbf{v}_M$$

$$=\int_V f(w)dw\,dw^*.$$

For an $I\times J$ matrix $M=(M^i_j)$ we define an $I^*\times J^*$ matrix M^* by

$$M^{*i^*}_{j^*}=\sigma(g(j),g(i)-g(j))(M^i_j)^*.$$

Proposition 4.7: We have

$$D(w^*/z^*)=D(w/z)^*,\quad D(w^*/z)=D(w/z^*)^*.$$

Moreover,

$$\Delta(w^*/z^*)=\sigma(g(I),g(J)-g(I))\Delta(w/z)^*,$$

$$\Delta(w^*/z)=\sigma(-g(I),g(J)+g(I))\Delta(w/z^*)^*.$$

Proof: By Propositions 3.4 we obtain the first two equalities. The last two equalities follow from Proposition A.3 in the Appendix.

Proposition 4.8: Suppose w is an analytic mapping from U to V. Then

$$\Delta\left(\frac{(w,w^*)}{(z,z^*)}\right)=\Delta\left(\frac{w}{z}\right)\Delta\left(\frac{w}{z}\right)^*=\left|\Delta\left(\frac{w}{z}\right)\right|^2.$$

Proof: By Proposition 4.7 and Proposition A.4 in the

Appendix we have

$$\Delta\left(\frac{(w,w^*)}{(z,z^*)}\right)=\sigma(g(I),\ -g(J)+g(I))\Delta\left(\frac{w}{z}\right)\Delta\left(\frac{w^*}{z^*}\right)$$

$$=\Delta\left(\frac{w}{z}\right)\Delta\left(\frac{w}{z}\right)^*=\left|\Delta\left(\frac{w}{z}\right)\right|^2.$$

Now, we define integration on the general superspace $Z=A_I$ (I is not necessarily even). Let U be a saturated domain in Z. We define integration on the doubling $\mathrm{dbl}(U)$ of U as well as on U.

Let $f\in A^{U}$ (resp. $A^{\mathrm{dbl}(U)}$) be a G^∞ function and $f(z,\zeta)=\Sigma f_{M;N^*}(z)(\zeta^N)^*\zeta^M$ [resp. $f(z,z^*,\zeta,\zeta^*)=\Sigma f_{M;N^*}(z,z^*)\zeta^{N^*}\zeta^M$] be its standard expansion. Here f is said to have a compact support, if every $f_{M;N^*}(z)$ [resp. $f_{M;N^*}(z,z^*)$] has a compact support on the body $b(U)$ [resp. $b(\mathrm{dbl}(U))$].

Definition 4.9: Let f be a G^∞ function on U [resp. $\mathrm{dbl}(U)$] with compact support. The (*Berezin*) *integral* of f on U [resp. $\mathrm{dbl}(U)$] is defined as

$$\int_U f(z,\zeta)dz\,dz^*\,d\zeta\,d\zeta^*=\int_{b(U)}f_{I_1;I_1^*}(z)dz\,dz^*,$$

$$\left(\text{resp.}\int_{\mathrm{dbl}(U)}f(z,z^*,\zeta,\zeta^*)dz\,dz^*\,d\zeta\,d\zeta^*\right.$$

$$\left.=\int_{b(U)}f_{I_1;I_1^*}(z,z^*)dz\,dz^*\right),$$

where $f_{I_1;I_1^*}$ is the top of f.

Proposition 4.10: Let f be a G^∞ function on U and let $\mathrm{dbl}(f)\in G^\infty(\mathrm{dbl}(U))$ be the unique extension of f to $\mathrm{dbl}(U)$. Then the integral of f on U is equal to the integral of $\mathrm{dbl}(f)$ on $\mathrm{dbl}(U)$.

Proof: Immediate from the fact that the tops of f and $\mathrm{dbl}(f)$ coincide on $b(U)$.

Theorem 4.11: Let I and J be G sets and U be a saturated domain in $Z=A_I$. Let $(w,w^*)=(w^j,w^{j^*},\eta^l,\eta^{l^*})$ be a G^∞ mapping of $\mathrm{dbl}(U)$ to $\mathrm{dbl}(W)$, where $W=A_J$. Suppose that (w,w^*) is one to one and its Jacobian $\Delta((w,w^*)/(z,z^*))$ is nonzero. Let $V=(w(\mathrm{dbl}(U)),w^*(\mathrm{dbl}(U)))$ and f be a G^∞ function on V with compact support. Then we have

$$\int_{\mathrm{dbl}(U)}f(w,w^*,\eta,\eta^*)\Delta\left(\frac{(w,w^*)}{(z,z^*)}\right)dz\,dz^*\,d\zeta\,d\zeta^*$$

$$=\epsilon\int_V f(w,w^*,\eta,\eta^*)dw\,dw^*\,d\eta\,d\eta^*,$$

where $\Delta((w,w^*)/(z,z^*))$ is the superdeterminant of

$$\begin{pmatrix}(\partial w^j(\partial z^i)^{-1}) & (\partial w^j(\partial z^{i^*})^{-1})\\ (\partial w^{*j}(\partial z^i)^{-1}) & (\partial w^{*j}(\partial z^{i^*})^{-1})\end{pmatrix}$$

and ϵ is 1 or -1 according as $b(\Delta((w,w^*)/(z,z^*)))$ is positive or negative on the body $b(U)$.

Proof: As we did in the proof of Theorem 7.4 in Ref. 1, the proof of this theorem can be reduced to the following five cases.

(i) $w^j=w^j(z,z^*)\in b(A)$ for $z\in b(U)=b(\mathrm{dbl}(U))$ and $j\in J_0\cup J_0^*$,

and $\eta^l=\zeta^l$ for $l\in J_1\cup J_1^*$.

(ii) $w^{j_0}=z^{j_0}+a(z,z^*)$ with $a(z,z^*)^2=0$,

$w^j=z^j$ for $j\neq j_0$, and $\eta^l=\zeta^l$.

(iii) $w^{j_0}=z^{j_0}+a(z,z^*)\zeta^K\zeta^{L^*}$ with $K\cup L^*\neq\phi$,

$K\subset I_1$, $L^*\subset I_1^*$, $w^j=z^j$ for $j\neq j_0$ and $\eta^l=\zeta^l$.

(iv) $w^j=z^j$ and $\eta^l=\Sigma_k a_k^l(z,z^*)\zeta^k$.

(v) $w^j=z^j$, $\eta^{l_0}=\zeta^{l_0}+a(z,z^*)\zeta^K\zeta^{L^*}$, where $K\subset I_1$, $L^*\subset I_1^*$, and $K\cup L^*\neq\{l_0\}$.

Proposition 4.6 covers case (i). In the other cases we can show the desired equality by direct calculations in the same way as in Ref. 1, and we omit them.

Proposition 4.12: Let $w=(w^k)$ be a G^∞ mapping of U to W. Then w uniquely determines a G^∞ mapping $\mathrm{dbl}(w)=(w,w^*)$ of $\mathrm{dbl}(U)$ to $\mathrm{dbl}(W)$, and the Jacobian of $\mathrm{dbl}(w)$ is equal to the unique extension of the Jacobian $\Delta((w,w^*)/(z,z^*))$ of w.

Proof: Clear from Proposition 3.10.

Combining Proposition 4.10, Theorem 4.11, and Proposition 4.12 we have the following theorem.

Theorem 4.13: Let I and J be G sets and U be a saturated domain in $Z=A_I$. Let $w=(w^j,\eta^l)$ be a G^∞ mapping of U to W, where $W=A_J$. Suppose that w is one to one and $\Delta((w,w^*)/(z,z^*))\neq 0$. Let $V=w(U)$ and f be a G^∞ function on V with compact support. Then we have

$$\int_U f(w,\eta)\Delta\left(\frac{(w,w^*)}{(z,z^*)}\right)dz\,dz^*\,d\zeta\,d\zeta^*$$

$$=\epsilon\int_V f(w,\eta)dw\,dw^*\,d\eta\,d\eta^*,$$

where ϵ is 1 or -1 according as $b(\Delta((w,w^*)/(z,z^*)))$ is positive or negative on the body $b(U)$.

Remark 4.14: If the mapping w is analytic in Theorem 4.13, then by Proposition 4.8 we see $\epsilon=1$.

APPENDIX: SOME PROPERTIES OF DETERMINANTS

Let I and J be G sets such that $|I|=|J|$ and $I\cup J$ is either even or odd. Let M be an $I\times J$ matrix over A.

Proposition A.1: Suppose i_1 and i_2 (resp. j_1 and j_2) are different elements in I (resp. J) such that $g(i_1)=g(i_2)$ [resp. $g(j_1)=g(j_2)$]. Let N be an $I\times J$ matrix such that $N_j^{i_2}=M_j^{i_2}+kM_j^{i_1}$ (resp. $N_{j_2}^i=M_{j_2}^i+kM_{j_1}^i$) and $N_j^i=M_j^i$ for $i\neq i_2$ (resp. $j\neq j_2$), where $k\in\mathbb{C}$. Then we have

$$\det M=\det N.$$

Proof: Easy from Proposition 3.5 and Proposition 3.15 of Ref. 6.

Proposition A.2: We have

$$\det M^T=\sigma(g(I),g(J)-g(I))\det M.$$

Proof: See the proof of Proposition 3.13 in Ref. 6.

We define an $I^*\times J^*$ matrix M^* by

$$M^{*i^*}_{j^*}=\sigma(g(j),g(i)-g(j))(M_j^i)^*.$$

Proposition A.3: We have

$$\det M^* = \sigma(g(J),g(I)-g(J))(\det M)^*.$$

Proof: We shall prove the assertion in the case where $I \cup J$ is even. Let $A[y,y^*]$ be the algebra over A generated by y^j with $j \in J \cup J^*$ subject to the following commutation relations (generalized Grassmann algebra over A):

$$y^j y^k = -\sigma(g(j),g(k))y^k y^j, \quad j,k \in J \cup J^*,$$

$$ay^j = \sigma(\alpha,g(j))y^j a, \quad \alpha \in G, \quad a \in A_\alpha, \quad j \in J \cup J^*.$$

The transposition $*$ of A is extended to $A[y,y^*]$ by

$$(y^j)^* = y^{j^*}, \quad (y^{j^*})^* = y^j \quad \text{for } j \in J.$$

A bijection $\pi: I \to J$ is extended to a bijection $\pi: I \cup I^* \to J \cup J^*$ by

$$\pi(i^*) = \pi(i)^* \quad \text{for } i \in I.$$

Now we can perform calculations as follows:

$$\begin{aligned}
&\det M^* \prod_{j^* \in J^*} y^{j^*} \\
&= \sum_\pi \prod_{i^* \in I^*} M^{*i^*}_{\pi(i^*)} y^{\pi(i^*)} = \sum_\pi \prod_{i^* \in I^*} y^{\pi(i^*)} (M^i_{\pi(i)})^* \\
&= \left(\sum_\pi \prod_{i \in I} M^i_{\pi(i)} y^{\pi(i)} \right)^* \\
&= \left(\det M \prod_{j \in J} y^j \right)^* = \prod_{j^* \in J^*} y^{j^*} (\det M)^* \\
&= \sigma(g(J),g(I)-g(J))(\det M)^* \prod_{j^* \in J^*} y^{j^*}.
\end{aligned}$$

This shows the desired equality. The odd case can be proved similarly.

Proposition A.4: Let I_1, I_2, J_1, and J_2 be G sets such that $i < k$ for $i \in I_1$ and $k \in I_2$, $j < l$ for $j \in J_1$ and $l \in J_2$ and $|I_1| = |J_1|$. Suppose $I = I_1 \cup I_2$ and $J = J_1 \cup J_2$ and let A, B, C, and D be $I_1 \times J_1$, $I_1 \times J_2$, $I_2 \times J_1$, and $I_2 \times J_2$ matrices, respectively.

Let M be an $I \times J$ matrix given by $M = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$. If $B = 0$ or $C = 0$, then

$$\det M = \sigma(g(J_1),g(I_2)-g(J_2))\det A \det D.$$

Proof: Taking indeterminates y^j satisfying suitable σ-commutativity, we have from the definition of determinant that

$$\begin{aligned}
\det M \prod_{j \in J} y^j &= \sum_\pi \prod_{i \in I} M^i_{\pi(i)} y^{\pi(i)} \\
&= \sum_{\pi'} \left(\prod_{i \in I_1} A^i_{\pi'(i)} y^{\pi'(i)} \prod_{k \in I_2} D^k_{\pi'(k)} y^{\pi'(k)} \right) \\
&= \det A \prod_{j \in J_1} y^j \det D \prod_{j \in J_2} y^j \\
&= \sigma(g(j_1),g(I_2)-g(J_2))\det A \det D \prod_{j \in J} y^j,
\end{aligned}$$

where π' ranges over all the bijections from I to J such that $\pi'(i) \in J_1$ if $i \in I_1$ and $\pi'(i) \in J_2$ if $i \in I_2$. The desired equality follows.

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Cohomology in connection space, family index theorem, and Abelian gauge structure

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Using the natural connection form on a principal bundle $P(M,G)$ and the bundle $\mathfrak{A}(\mathfrak{A}/\mathcal{G},\mathcal{G})$ a systematic derivation of the double-cohomological series constituted by the exterior differential d on space-time M and arbitrary, horizontal, and vertical variations in connection space is given. The relationship between these cohomologies and the family index theorem is clarified. The formalism is then used to analyze Abelian gauge structure inside non-Abelian gauge theory. The pertinent functional $U(1)$ connection form, curvature form, and three-form "curvature" are identified and computed, and are related to the θ vacuum, anomalous commutation relation, and Jacobi identity, respectively. Some of the results differ from those obtained by Wu and Zee [Nucl. Phys. B **258**, 157 (1985)] and Niemi and Semenoff [Phys. Rev. Lett. **55**, 227 (1985)] and the results of this paper recover theirs under certain conditions. Finally the generalization of the formalism to a nontrivial principal bundle by introduction of a fixed background connection form is discussed.

I. INTRODUCTION

Recently there has been active interest in anomalies[1–5] in quantum theory. The cohomology of Lie algebras and Lie groups has been discussed by a number of authors. Bonora *et al.*,[6] Stora,[7] and Zumino[8] give the descent equation of the gauge algebra δ_v and the exterior differential d. Faddeev[9] discusses the double-cohomological series of the transformation Δ_v of the gauge group and d. Zumino[10] shows that the cohomology of the gauge group can be reduced to that of its Lie algebra.

If we describe the connection space $\mathfrak{A}$ as a fiber bundle with $\mathfrak{A}/\mathcal{G}$ as the base and $\mathcal{G}$ as the structure group, the variation $\delta_v(\Delta_v)$ is the one along the fiber $\mathcal{G}$. The corresponding cohomology is called the vertical one. On the other hand, Gelfand[11] and Faddeev *et al.*[12] introduce the horizontal variation $\delta_h(\Delta_h)$ along the base $\mathfrak{A}/\mathcal{G}$, and establish the descent equation of $\delta_h(\Delta_h)$ and d. We call the cohomology associated with $\delta_h(\Delta_h)$ the horizontal one. In addition to these cohomologies, Guo *et al.*[13] first discuss the cohomological series of d and the interpolation variation in the connection space $\mathfrak{A}$.

However, few attempts have been made to study the relationship between the horizontal and vertical cohomologies, which seem to be different. Faddeev[12] and Hou *et al.*[14] claim that they have given the relationship between these cohomologies. Since the operations of Δ_v and Δ_h do not match each other, the relation they obtain in their paper is very complicated and not obvious. A deep understanding of the relationship between horizontal and vertical cohomologies is still lacking. In addition, one may ask the following question: What is the relationship between these cohomologies and the family index theorem?

This paper is a modest attempt to try to answer these questions. Using the natural connection form on a principal bundle $P(M,G)$ and bundle $\mathfrak{A}(\mathfrak{A}/\mathcal{G},\mathcal{G})$ we deal with an arbitrary variation δ, a horizontal one δ_h, and vertical one δ_v in a unified point of view. We also give a systematical derivation of the generalized finite double-cohomological series in the space of all connection forms. We show very simple and obvious relations between horizontal and vertical cohomologies and, in particular, between these cohomologies and the family index theorem.[15,16]

As an application of our formalism, we examine the Abelian gauge structure inside non-Abelian gauge theory. This has been discussed first by Jackiw[17] and then by Wu *et al.*[18] and Niemi *et al.*[19] They compute the functional $U(1)$ connection form and curvature form on connection space by using the path integral formulation, the Hamiltonian formulation, and the η invariant of Dirac operator, respectively. In this paper we obtain the results in their works in a different way by using the family index theorem and cohomology in connection space. We also obtain some new results that reduce to those in Refs. 18 and 19 under certain conditions.

This paper will be organized as follows: In Sec. II we discuss three kinds of cohomological series on connection space, the family index theorem, and the relations among them. In Secs. III–V, we present the application of our formalism to examining Abelian gauge structure inside non-Abelian gauge theory. Section VI is devoted to the generalization of our formalism to nontrivial principal bundle. In Sec. VII we give some conclusions and discussions.

II. THE FORMALISM

Consider connection forms on compactified Euclidean space-time M. We shall first assume the principal bundle $P(M,G)$ has trivial topology, i.e., $P=M\times G$, where G is a semisimple Lie group. (The case that principal bundle is nontrivial will be discussed in Sec. VI.) Let $\mathfrak{A}$ be the set of all such connection forms, $\mathfrak{A}=\{A(x)\}$. Let $\mathcal{G}$ be the gauge group, i.e., the set of maps $g: M\to G\,(x\mapsto g(x))$, $\mathcal{G}=\{g(x)\}$. Let $\mathfrak{A}/\mathcal{G}$ be the corresponding orbit space, that is, the set of different orbits. Because $\mathcal{G}$ is nontrivial, $\mathfrak{A}/\mathcal{G}$ has a topology. In fiber bundle language, the connection space $\mathfrak{A}$ may be described as a fiber bundle with $\mathfrak{A}/\mathcal{G}$ as base and $\mathcal{G}$ as struc-

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ture group. Following Stora,[7] we can locally parametrize $\mathfrak{A}$ by

$$A = g^{-1}ag + g^{-1}\,dg, \tag{2.1}$$

where a represents an orbit. Then a cotangent vector in $\mathfrak{A}$ is

$$\delta A = g^{-1}\delta a g - D_A(g^{-1}\delta g) \quad \text{with } D_A \equiv d + [A,\ ]. \tag{2.2}$$

We can introduce on $\mathfrak{A}$ the connection form

$$\mathscr{A} = -G_A D_A^{+}\delta A \quad \text{with } G_A \equiv (D_A^{+}D_A)^{-1} \tag{2.3}$$

so that

$$\mathscr{A}|_{\text{fiber}} = g^{-1}\delta_v g. \tag{2.4}$$

Here δA can be decomposed into a horizontal component $\delta_h A$ and a vertical one $\delta_v A$,

$$\begin{aligned}\delta_h A &= (1 - D_A G_A D_A^{+})\delta A,\\ \delta_v A &= D_A G_A D_A^{+}\delta A = -D_A\mathscr{A}.\end{aligned} \tag{2.5}$$

The total connection form over $M\times\mathfrak{A}/\mathscr{G}$ at $(g(x),g(\cdot);x,A)$ is

$$A + \mathscr{A} = A - G_A D_A^{+}\delta A. \tag{2.6}$$

The corresponding curvature form is

$$\begin{aligned}\mathscr{F} &= (d+\delta)(A+\mathscr{A}) + \tfrac{1}{2}[A+\mathscr{A}, A+\mathscr{A}]\\ &= F + \delta_h A + (\delta\mathscr{A} + \mathscr{A}^2)\\ &= F + (\mathscr{F})_1^1 + (\mathscr{F})_0^2,\end{aligned} \tag{2.7}$$

where $F = dA + \frac{1}{2}[A,A]$ and $(\ )_j^i$ stands for a j-form on P and i-form on $\mathfrak{A}$.

The bundle and connections can be pulled back onto $M\times\mathfrak{A}/\mathscr{G}$. According to the family index theorem,[15] the characteristic classes on $\mathfrak{A}/\mathscr{G}$ are expressible as integral of the higher classes on $M\times\mathfrak{A}/\mathscr{G}$ over the base M:

$$Q^k(M) = \int_M P_{2n}(\mathscr{F}^n), \tag{2.8}$$

forms of degree k on $\mathfrak{A}/\mathscr{G}$, where $P_{2n}(\mathscr{F}^n)$ is an n-rank invariant polynomial in $\mathscr{F}$ and the dimension of M is $(2n-k)$. We can choose locally horizontal gauge[12] $D_A^{+}\delta A = 0$ such that $\mathscr{A} = 0$. It is convenient to define space in which $\mathscr{A} = 0$ as $\mathfrak{A}/\mathscr{G}$. So, from Eq. (2.7) we obtain $\mathscr{F}$ in horizontal gauge and we denote it by $\hat{\mathscr{F}}$,

$$\hat{\mathscr{F}} = F + \delta_h A = (d+\delta_h)A + \tfrac{1}{2}[A,A]. \tag{2.9}$$

The Bianchi identity $D_h\hat{\mathscr{F}} \equiv (d+\delta_h)\hat{\mathscr{F}} + [A,\hat{\mathscr{F}}] = 0$ implies that

$$(d+\delta_h)P_{2n}(\hat{\mathscr{F}}^n) = 0. \tag{2.10}$$

Expanding the $P_{2n}(\hat{\mathscr{F}}^n)$,

$$P_{2n}(\hat{\mathscr{F}}^n) = \sum_k q_{2n-k}^k(F,\delta_h A), \tag{2.11}$$

we have the following descent equation:

$$\begin{aligned}&dq_{2n}^0(F,\delta_h A) = 0, \quad \delta_h q_0^{2n}(F,\delta_h A) = 0,\\ &dq_{2n-k}^k(F,\delta_h A) = -\delta_h q_{2n-k+1}^{k-1}(F,\delta_h A).\end{aligned} \tag{2.12}$$

Introducing integration over an arbitrary nonclosed k-chain $\hat{\Delta}^k$ in $\mathfrak{A}/\mathscr{G}$,

$$\hat{Q}_{2n-k}(\hat{\Delta}^k) = \int_{\hat{\Delta}^k} q_{2n-k}^k(F,\delta_h A) \tag{2.13}$$

and over an arbitrary $(2n-k)$-chain C_{2n-k} in space-time M,

$$\hat{Q}^k(C_{2n-k}) = \int_{C_{2n-k}} q_{2n-k}^k(F,\delta_h A), \tag{2.14}$$

we obtain the following finite double-cohomological series from Eq. (2.12) and the Stokes theorem:

$$d\hat{Q}_{2n-k-1}(\hat{\Delta}^{k+1}) = -\hat{Q}_{2n-k}(\partial_h\hat{\Delta}^{k+1}), \tag{2.15a}$$

$$\delta_h\hat{Q}^{k-1}(C_{2n-k+1}) = -\hat{Q}^k(\partial C_{2n-k+1}). \tag{2.15b}$$

Here ∂_h denotes the boundary operation in $\mathfrak{A}/\mathscr{G}$. The Chern classes associated with the family index, when a locally horizontal gauge is chosen, are given by Eq. (2.14) and satisfy the descent equation (2.15b) for horizontal variation δ_h and exterior differential d. Note that when $\hat{\Delta}$ is a simplex, Eq. (2.15b) reduces to the double-cohomological series given by Faddeev.[12]

It follows from Eq. (2.15b) that

$$\delta_h\hat{Q}^k(M_{2n-k}) = 0, \quad \text{when } \partial M_{2n-k} = 0. \tag{2.16}$$

However, $\hat{Q}^k(M_{2n-k}) \neq \delta_h$ (something) because of nontriviality of the base space $\mathfrak{A}/\mathscr{G}$.

The Chern classes $\hat{Q}^k(M_{2n-k})$, which are k-forms on $\mathfrak{A}/\mathscr{G}$, can be lifted to k-forms $Q^k(M_{2n-k})$ on $\mathfrak{A}$. In order to do this, we first lift the $q_{2n-k}^k(F,\delta_h A)$ to $\mathfrak{A}$ and obtain

$$q_{2n-k}^k(\mathscr{F}^n) = \sum_{\substack{l_1,\dots,l_n=0\\ l_1+\cdots+l_n=k}}^{2} P_{2n}((\mathscr{F})_{2-l_1}^{l_1},\dots,(\mathscr{F})_{2-l_n}^{l_n}). \tag{2.17}$$

Invariance of the $P_{2n}(\mathscr{F}^n)$, i.e., $(d+\delta)P_{2n}(\mathscr{F}^n) = 0$, gives

$$\begin{aligned}&dq_{2n}^0(\mathscr{F}^n) = 0, \quad \delta q_0^{2n}(\mathscr{F}^n) = 0,\\ &dq_{2n-k}^k(\mathscr{F}^n) = -\delta q_{2n-k+1}^{k-1}(\mathscr{F}^n).\end{aligned} \tag{2.18}$$

We can thus construct k-forms on $\mathfrak{A}$,

$$Q^k(C_{2n-k}) = \int_{C_{2n-k}} q_{2n-k}^k(\mathscr{F}^n), \tag{2.19}$$

and $(2n-k)$-forms on M,

$$Q_{2n-k}(\Delta^k) = \int_{\Delta^k} q_{2n-k}^k(\mathscr{F}^n), \tag{2.20}$$

where the C_{2n-k} are arbitrary $(2n-k)$-chains in space-time M and Δ^k k-chains in $\mathfrak{A}$. We can easily show from Eq. (2.18) and the Stokes theorem that

$$dQ_{2n-k-1}(\Delta^{k+1}) = -Q_{2n-k}(\partial\Delta^{k+1}), \tag{2.21a}$$

$$\delta Q^{k-1}(C_{2n-k+1}) = -Q^k(\partial C_{2n-k+1}). \tag{2.21b}$$

These are double-cohomological series in the space $\mathfrak{A}$.

According to the family index theorem,[15] the $Q^k(C_{2n-k})$, defined on $\mathfrak{A}$, defines a k-form on $\mathfrak{A}/\mathscr{G}$. This can be proved[7] by checking that the term $-D_A(g^{-1}\delta g)$ in δA does not contribute to the result (up to d of some form) if we look at the nonintegrated $q_{2n-k}^k(\mathscr{F}^n)$. This observation is important when we exmine the global property of horizontal cohomology.

We obviously have from Eq. (2.21)

$$\delta Q^k(M_{2n-k}) = 0 \quad \text{when } \partial M_{2n-k} = 0, \tag{2.22}$$

which shows that the $Q^k(M_{2n-k})$ are cocycles on $\mathfrak{A}$. The

$Q^k(M_{2n-k})$ are also exact since $\mathfrak{A}$ has no topology, that is,

$$Q^k(M_{2n-k}) = \delta\Omega^{k-1}(M_{2n-k}). \tag{2.23}$$

Here $\Omega^{k-1}(M_{2n-k})$ can be determined as follows: Since the principal bundle has trivial topology, we obtain from the relation that

$$(d+\delta)P_{2n}(\mathscr{F}^n) = 0$$

that

$$P_{2n}(\mathscr{F}^n) = (d+\delta)\omega_{2n-1}(A+\mathscr{A}). \tag{2.24}$$

Here $\omega_{2n-1}(A+\mathscr{A})$ is given by the well-known transgression formula due to Chern,

$$\omega_{2n-1}(A+\mathscr{A}) = n\int_0^1 dt\, P_{2n}(A+\mathscr{A},\mathscr{F}_t^{n-1}) \tag{2.25}$$

with $\mathscr{F}_t = t\mathscr{F} + (t^2-t)(A+\mathscr{A})^2$.

Integrating Eq. (2.24) over M_{2n-k} without boundary and then comparing it with Eq. (2.23) we obtain

$$Q^k(M_{2n-k}) = \int_{M_{2n-k}} q^k_{2n-k}(\mathscr{F}^n), \tag{2.26}$$

$$\Omega^{k-1}(M_{2n-k}) = \int_{M_{2n-k}} \omega^{k-1}_{2n-k}(A;\mathscr{A}), \tag{2.27}$$

where $\omega^k_{2n-k}(A;\mathscr{A})$ stands for the $(2n-k,k-1)$ component of the $\omega_{2n-1}(A+\mathscr{A})$.

When limited to fiber, Eq. (2.24) becomes

$$P_{2n}(\breve{\mathscr{F}}^n) = P_{2n}(F^n) = (d+\delta v)\breve{\omega}_{2n-1}(A+v), \tag{2.28}$$

where use has been made of the following facts:

$$\begin{aligned} &\mathscr{A}|_{\text{fiber}} \equiv \breve{\mathscr{A}} = g^{-1}\delta_v g \equiv v, \quad \mathscr{F}|_{\text{fiber}} \equiv \breve{\mathscr{F}} = F, \\ &\omega_{2n-1}(A+\mathscr{A})|_{\text{fiber}} \equiv \breve{\omega}_{2n-1}(A+v). \end{aligned} \tag{2.29}$$

Expanding the $\breve{\omega}_{2n-1}(A+v)$ in v:

$$\breve{\omega}_{2n-1}(A+v) = \sum_k \breve{\omega}^k_{2n-k}(v;A). \tag{2.30}$$

We obtain from Eq. (2.28):

$$\begin{aligned} &d\breve{\omega}^0_{2n-1}(v;A) = q^0_{2n}(F^n) = P_{2n}(F^n), \\ &\delta_v\breve{\omega}^{2n-1}_0(v;A) = 0, \\ &\delta_v\breve{\omega}^{k-1}_{2n-k}(v;A) = -d\breve{\omega}^k_{2n-k-1}(v;A). \end{aligned} \tag{2.31}$$

Introducing the integrations

$$\breve{\Omega}^k(C_{2n-k-1}) = \int_{C_{2n-k-1}} \breve{\omega}^k_{2n-k-1}(v;A), \tag{2.32}$$

$$\breve{\Omega}_{2n-k-1}(\Gamma^k) = \int_{\Gamma^k} \breve{\omega}^k_{2n-k-1}(v;A), \tag{2.33}$$

where the Γ^k are arbitrary k-chains in $\mathscr{G}$, we have the following finite double-cohomological series from Eq. (2.31) and the Stokes theorem:

$$d\breve{\Omega}_{2n-k-1}(\Gamma^k) = -\breve{\Omega}_{2n-k}(\partial_v\Gamma^k), \tag{2.34a}$$

$$\delta_v\breve{\Omega}^{k-1}(C_{2n-k}) = -\breve{\Omega}^k(\partial C_{2n-k}), \tag{2.34b}$$

where ∂_v stands for the boundary operation in $\mathscr{G}$. When Γ^k is a simplex, Eq. (2.34a) reduces to the $\Delta_v - d$ series given by Faddeev.[9]

Now the relation between the horizontal and the vertical cohomologies, and in particular between these cohomologies and the family index theorem, may be formulated: Introduce integrations

$$\alpha(\Gamma^k, C_{2n-k-1}) = \int_{\Gamma^k} \Omega^k(C_{2n-k-1}), \tag{2.35}$$

$$Q(\Delta^{k+1}, C_{2n-k-1}) = \int_{\Delta^{k+1}} Q^{k+1}(C_{2n-k-1}). \tag{2.36}$$

We choose the $(k+1)$-chains Δ^{k+1} in such a way that their boundaries belong to $\mathscr{G}$, i.e., $\partial\Delta^{k+1} = \Gamma^k \in \mathscr{G}$, and the projection of Δ^{k+1} into $\mathfrak{A}/\mathscr{G}$ is a k-dimensional sphere S^k in it. Noticing that

$$\Omega^k(M_{2n-k-1})|_{\text{fiber}} = \breve{\Omega}^k(M_{2n-k-1}), \tag{2.37}$$

we can easily show by means of Eq. (2.23) that

$$Q(\Delta^{k+1}, C_{2n-k-1}) = \alpha(\Gamma^k, C_{2n-k-1}), \tag{2.38}$$

and, in particular,

$$\begin{aligned} \pi^{k+1}(\mathfrak{A}/\mathscr{G}) &= Q(\Delta^{k+1}, M_{2n-k-1}) \\ &= \alpha(\Gamma^k, M_{2n-k-1}) = \pi^k(\mathscr{G}). \end{aligned} \tag{2.39}$$

We have thus linked the horizontal and vertical cohomologies with the family index theorem.

The above analyses are general and abstract. To further understand the formalism requires a concrete calculation, which we will carry out in the following sections.

III. U(1) CONNECTION FORM ON $\mathfrak{A}$ AND θ VACUUM

As a first application of the above formalism, we consider the $(3+1)$-dimensional gauge theory without non-Abelian anomaly.[20] Fix gauge $A_0 = 0$ and consider the space $\mathfrak{A}^3$ of all static gauge field configurations $A^a_i(\vec{x})$. In the Schrödinger formulation the wave functional is $\psi[A]$. The Gauss law

$$D_i(\delta/\delta A^a_i)\psi[A] = 0 \tag{3.1}$$

can be used to eliminate the residual static gauge freedom, $D_i(\delta/\delta A^a_i)$ is an infinitesimal generator of the gauge transformation. In the homotopically trivial case a finite gauge transformation can be obtained from an infinitesimal one. Therefore the Gauss law means that the wave functional $\psi[A]$ is invariant under "small" gauge transformations. Here the so-called small gauge transformations are those that can be obtained from the identity by infinitesimal ones. We know that there are "large" gauge transformations that cannot be obtained in this way in the homotopically nontrivial case. The wave functional is not invariant under large transformations

$$\psi[A^g] = e^{in\theta}\psi[A] \quad (A^g = g^{-1}Ag + g^{-1}dg). \tag{3.2}$$

From the discussions in the above section we can easily compute the one-form on $\mathfrak{A}^3/\mathscr{G}^3$:

$$\begin{aligned} \hat{Q}^1(S^3) &= \int_{S^3} q^1_3(F, \delta_h A) \\ &= -\frac{1}{8\pi^2}\int_{S^3} (\mathrm{tr}(F+\delta_h A)^2)^1_3 \\ &= -\frac{1}{4\pi^2}\int_{S^3} \mathrm{tr}(F\delta_h A), \end{aligned} \tag{3.3}$$

which is closed, i.e., $\delta_h \hat{Q}^1(S^3) = 0$, but not exact. We can lift $\hat{Q}^1(S^3)$ and obtain a one-form on $\mathfrak{A}^3$:

$$\begin{aligned} Q^1(S^3) &= \int_{S^3} q_3^1(\mathscr{F}^2) \\ &= -\frac{1}{8\pi^2}\int_{S^3} \mathrm{tr}((\mathscr{F})_1^1 F) + \mathrm{tr}(F(\mathscr{F})_1^1) \\ &= -\frac{1}{4\pi^2}\int_{S^3} \mathrm{tr}(F(\mathscr{F})_1^1) \\ &= -\frac{1}{4\pi^2}\int_{S^3} \mathrm{tr}(F\delta A). \end{aligned} \tag{3.4}$$

We can explain $Q^1(S^3)$ as a $U(1)$ connection form on $\mathfrak{A}^3$. The corresponding curvature two-form is

$$\begin{aligned} \delta Q^1(S^3) &= -\frac{1}{4\pi^2}\int_{S^3} \mathrm{tr}(\delta A \delta A) \\ &= \frac{1}{4\pi^2}\int_{S^3} \mathrm{tr}(\delta A D_A(\delta A)) \\ &= \frac{1}{2\pi^2}\int_{S^3} d(\mathrm{tr}(\delta A \delta A)) = 0. \end{aligned} \tag{3.5}$$

Therefore the field strength form of the $U(1)$ potential form is zero. Equations (3.4) and (3.5) are the $U(1)$ connection and the curvature form given by Wu and Zee,[18] respectively. We have obtained these anew using our formalism.

Since base $\mathfrak{A}^3$ has the trivial topology, Eq. (3.5) means that $Q^1(S^3)$ is also exact on $\mathfrak{A}^3$, i.e.,

$$Q^1(S^3) = \delta\Omega^0(S^3) \tag{3.6a}$$

with $\Omega^0(S^3)$ given by Eq. (2.27):

$$\begin{aligned} \Omega^0(S^3) &= \int_{S^3} \omega_3^0(A + \mathscr{A}) \\ &= -\frac{1}{4\pi^2}\int_{S^3}\int_0^1 dt(\mathrm{tr}((A + \mathscr{A})\mathscr{F}_t))_3^0 \\ &= -\frac{1}{8\pi^2}\int_{S^3} \mathrm{tr}(A\,dA + \tfrac{2}{3}A^3). \end{aligned} \tag{3.6b}$$

Thus the connection form $Q^1(S^3)$ is a pure gauge.

Now we consider integration of the potential one-form $Q^1(S^3)$ over an open path Δ^1 in $\mathfrak{A}^3$. Let its boundary be two points A^g and A on the same gauge orbit. Then from Eq. (3.6),

$$\begin{aligned} \int_{\Delta^1} Q^1(S^3) &= \int_{\Delta^1} \delta\Omega^0(S^3) = \int_{\partial\Delta^1} \Omega^0(S^3) = \int_{\Gamma^0} \Omega^0(S^3) \\ &= -\frac{1}{8\pi^2}\int_{S^3} (\mathrm{tr}(A^g\,dA^g + \tfrac{2}{3}(A^g)^3) \\ &\quad - \mathrm{tr}(A\,dA + \tfrac{2}{3}A^3)) \\ &= -\frac{1}{24\pi^2}\int_{S^3} \mathrm{tr}(g^{-1}\,dg)^3 = Z. \end{aligned} \tag{3.7}$$

The above equation is an explicit manifestation of the relation $\pi^1(\mathfrak{A}^3/\mathscr{G}^3) = \pi^0(\mathscr{G}^3) = Z$, which shows that there exist noncontractible loops in $\mathfrak{A}^3/\mathscr{G}^3$. We thus have vortex field in $\mathfrak{A}^3/\mathscr{G}^3$, in agreement with the conclusion in Ref. 18.

If we define

$$\Phi[A] = \exp\left(\frac{1}{8\pi^2}\int_{S^3} \mathrm{tr}\left(A\,dA + \frac{2}{3}A^3\right)\theta\right)\chi[A], \tag{3.8}$$

$\Phi[A]$ is gauge invariant from Eqs. (3.2) and (3.7). However, in quantum theory a phase change in the wave functional corresponds to a canonical transformation,[17] which will induce a change in the Lagrangian by a total derivative, and therefore leads to the vacuum θ angle in the Yang–Mills Lagrangian.

IV. U(1) CURVATURE FORM AND ANOMALOUS COMMUTATOR ON $\mathfrak{A}$

In this section, we shall consider non-Abelian gauge theory[21] defined on space-time manifold S^3. We shall fix $A_0 = 0$ and consider the infinite-dimensional affine space $\mathfrak{A}^2$ of all static gauge field configurations $A_i^a(\vec{x})$. The two-form on $\mathfrak{A}^2/\mathscr{G}^2$ is

$$\begin{aligned} \hat{Q}^2(S^2) &= \int_{S^2} q_2^2(F, \delta_h A) = -\frac{1}{8\pi^2}\int_{S^2} (\mathrm{tr}(F + \delta_h A)^2)_2^2 \\ &= -\frac{1}{8\pi^2}\int_{S^2} \mathrm{tr}(\delta_h A \delta_h A). \end{aligned} \tag{4.1}$$

Lifting $\hat{Q}^2(S^2)$, we obtain a two-form on $\mathfrak{A}^2$,

$$\begin{aligned} Q^2(S^2) &= \int_{S^2} q_2^2(\mathscr{F}^2) \\ &= -\frac{1}{8\pi^2}\int_{S^2} (\mathrm{tr}(\mathscr{F}^2))_2^2 = -\frac{1}{4\pi^2}\int_{S^2} \mathrm{tr}((\mathscr{F})_0^2 F) \\ &\quad -\frac{1}{8\pi^2}\int_{S^2} \mathrm{tr}((\mathscr{F})_1^1(\mathscr{F})_1^1) \\ &= -\frac{1}{8\pi^2}\int_{S^2} \mathrm{tr}(\delta A \delta A) - \frac{1}{4\pi^2}\delta\int_{S^2} \mathrm{tr}(\mathscr{A}F), \end{aligned} \tag{4.2}$$

which is obviously closed: $\delta Q^2(S^2) = 0$. Here $Q^2(S^2)$ can be identified as the $U(1)$ curvature two-form on $\mathfrak{A}^2$. The $Q^2(S^2)$ is also exact because of topological triviality of the space $\mathfrak{A}^2$:

$$Q^2(S^2) = \delta\Omega^1(S^2), \tag{4.3a}$$

where

$$\begin{aligned} \Omega^1(S^2) &= \int_{S^2} \omega_2^1(A + \mathscr{A}) \\ &= -\frac{1}{4\pi^2}\int_{S^2}\int_0^1 \mathrm{dt}(\mathrm{tr}((A + \mathscr{A})\mathscr{F}_t))_2^1 \\ &= -\frac{1}{8\pi^2}\int_{S^2} \mathrm{tr}(A\delta A) - \frac{1}{4\pi^2}\int_{S^2} \mathrm{tr}(\mathscr{A}F). \end{aligned} \tag{4.3b}$$

Thus we have obtained the connection one-form $\Omega^1(S^2)$ on $\mathfrak{A}^2$. Note that when $\mathscr{A} = 0$, only the first term in Eq. (4.2) and (4.3b) survives: This corresponds to the expressions obtained by Wu and Zee.[18]

Now let us examine the integration of $Q^2(S^2)$ over a two-dimensional disk Δ^2 in $\mathfrak{A}^2$. Assume its boundary $\partial\Delta^2 = \Gamma^1$ is a one-dimensional loop in $\mathscr{G}^2$. We then have from Eq. (4.3)

$$\int_{\Delta^2} Q^2(S^2) = \int_{\Delta^2} \delta\Omega^1(S^2) = \int_{\partial\Delta^2} \Omega^1(S^2) = \int_{\Gamma^1} \Omega^1(S^2)$$
$$= \int_{\Gamma^1} \breve{\Omega}^1(S^2) = \int_{\Gamma^1}\int_{S^2} \breve{\omega}_2^1$$
$$= \int_{\Gamma^1_+}\int_{S^2} \breve{\omega}_2^1 - \int_{\Gamma^1_-}\int_{S^2} \breve{\omega}_2^1$$
$$= \int_{\Gamma^0}\int_{D^3_+} \breve{\omega}_3^0 - \int_{\Gamma^0}\int_{D^3_-} \breve{\omega}_3^0 = \int_{\Gamma^0}\int_{S^3} \breve{\omega}_3^0 = Z. \tag{4.4}$$

Therefore the Chern number associated with a functional $U(1)$ connection form $\Omega^1(S^2)$ is an integer n, in contrast to the conclusion in Ref. 18. Note that Eq. (4.4) means that $\pi^2(\mathfrak{A}^2/\mathcal{G}^2) = \pi^1(\mathcal{G}^2) = Z$, which shows that there exists a noncontractible two-dimensional sphere in $\mathfrak{A}^2/\mathcal{G}^2$. So, we have a monopole in the orbit space $\mathfrak{A}^2/\mathcal{G}^2$.[18]

The above system, quantized in Schrödinger formulation, is the infinite-dimensional version of quantum electrodynamics in ordinary space, and as in the finite case, the field velocity operator

$$V_X = \delta_X + \Omega^1(S^2), \quad \delta_X = \int d^2x\, \delta A_i^a(x) \frac{\delta}{\delta A_i^a(x)}, \tag{4.5}$$

on $\mathfrak{A}^2$ describes a gauge field (where X stands for sum over a, i, and integration over $\vec{x}$) for an external $U(1)$ connection form $\Omega^1(S^2)$. The commutation relation leads to the nonzero curvature two-form

$$[V_X, V_Y] = \delta\Omega^1(S^2) = Q^2(S^2)$$
$$= -\frac{1}{8\pi^2}\int_{S^2} \mathrm{tr}(\delta A \delta A) - \frac{1}{4\pi^2}\delta\int_{S^2} \mathrm{tr}(\mathscr{A}F), \tag{4.6}$$

which, being independent of the dynamical variable, satisfies the Jacobi identity

$$[V_X,[V_Y,V_Z]] + (\text{perm.}) = \delta Q^2(S^2) = 0. \tag{4.7}$$

Thus the translations (i.e., field velocity operators) on $\mathfrak{A}^2$ constitute a Lie group. However, the Gauss law fails because V_X satisfies anomalous commutation relation.

V. FUNCTIONAL U(1) GAUGE THEORY WITHOUT A CONNECTION ONE-FORM AND THE ANOMALOUS JACOBI IDENTITY ON $\mathfrak{A}$

We now consider $(3+1)$-dimensional gauge theory with non-Abelian anomaly.[1] Assume a non-Abelian gauge field is minimally coupled to Weyl fermions in a complex representation of some gauge group. We once again fix $A_0 = 0$ and consider the infinite-dimensional affine space $\mathfrak{A}^3$ of all static gauge field configurations $A_i^a(x)$. Form $\mathfrak{A}^3/\mathcal{G}^3$, the space of three-dimensional gauge fields modulo three-dimensional gauge transformations. Since we are dealing with anomalous gauge theory, we have to consider a two-form on $\mathfrak{A}^3$. To this end, we first compute a three-form on $\mathfrak{A}^3/\mathcal{G}^3$. We have, from Eq. (2.14),

$$\hat{Q}^3(S^3) = \int_{S^3} q_3^3(F,\delta_h A) = -\frac{i}{48\pi^3}\int_{S^3} (\mathrm{tr}(F+\delta_h A)^3)_3^3$$
$$= -\frac{i}{48\pi^3}\int_{S^3} \mathrm{tr}(\delta_h A \delta_h A \delta_h A). \tag{5.1}$$

This form is closed, i.e., $\delta_h \hat{Q}^3(S^3) = 0$, but not exact. In order to relate to anomaly, we lift the $\hat{Q}^3(S^3)$ and derive a three-form on $\mathfrak{A}^3$:

$$Q^3(S^3) = \int_{S^3} q_3^3(\mathscr{F}^3) = -\frac{i}{48\pi^3}\int_{S^3} (\mathrm{tr}\,\mathscr{F}^3)_3^3$$
$$= -\frac{i}{48\pi^3}\int_{S^3} \mathrm{tr}((\mathscr{F})_1^1)^3 - \frac{i}{16\pi^3}\int_{S^3} \mathrm{tr}((\mathscr{F})_1^1(\mathscr{F})_0^2 F) - \frac{i}{16\pi^3}\int_{S^3} \mathrm{tr}((\mathscr{F})_0^2(\mathscr{F})_1^1 F)$$
$$= -\frac{i}{48\pi^3}\int_{S^3} \mathrm{tr}(\delta A \delta A \delta A) - \frac{i}{16\pi^3}\delta\int_{S^3} \mathrm{tr}(F\delta A\mathscr{A} + F\mathscr{A}\delta A + F\mathscr{A}D_A\mathscr{A}). \tag{5.2}$$

This is also closed: $\delta Q^3(S^3) = 0$. Notice that the $Q^3(S^3)$ is exact on $\mathfrak{A}^3$ because of its topological triviality

$$Q^3(S^3) = \delta\Omega^2(S^3). \tag{5.3a}$$

The two-form $\Omega^2(S^3)$ is given by Eq. (2.27),

$$\Omega^2(S^3) = \int_{S^3} \omega_3^2(A+\mathscr{A}) = -\frac{i}{16\pi^3}\int_{S^3}\int_0^1 dt(\mathrm{tr}((A+\mathscr{A})\mathscr{F}_t^2))_3^2$$
$$= -\frac{i}{48\pi^3}\int_{S^3} \mathrm{tr}(A\delta A\delta A) - \frac{i}{16\pi^3}\int_{S^3} \mathrm{tr}(F\delta A\mathscr{A} + F\mathscr{A}\delta A + F\mathscr{A}D_A\mathscr{A}) - \frac{i}{16\pi^3}\delta\int_{S^3} \mathrm{tr}\left(\mathscr{A}\left(AF + FA - \frac{1}{2}A^3\right)\right). \tag{5.3b}$$

We can identify $\Omega^2(S^3)$ and $Q^3(S^3)$ with the generalized functional $U(1)$ "potential" two-form and "field strength" three-form on $\mathfrak{A}^3$, respectively. Therefore, the system, quantized in the Schrödinger formulation, is an infinite-dimensional version of a quantum mechanical point particle that moves in a background field without potential one-form as discussed by Hou *et al.* in Ref. 22. We have to deal with the functional $U(1)$ antisymmetrical tensor gauge theory[23] without potential one-form. Such a system shares many features with quantum electrodynamics without potential in ordinary space-time: First there is no smooth $U(1)$ potential one-form on $\mathfrak{A}^3$. Second the representation space of the translation group acting on $\mathfrak{A}^3$ is not ordinary functional Hilbert space, and we have to introduce a membrane-dependent wave functional[22] on $\mathfrak{A}^3$. So, we have the situation as in Mandelstam.[24] In analogy with the finite-dimensional case

covariant translations on $\mathfrak{A}^3$ are generated by the "velocity" operator (or so-called electric field) E_X,[19] although it is not a smooth functional. The commutation relation gives the "connection" two-form

$$[E_X,E_Y]=\Omega^2(S^3)=-\frac{i}{48\pi^3}\int_{S^3}\mathrm{tr}(A\delta A\delta A)$$
$$-\frac{i}{16\pi^3}\int_{S^3}\mathrm{tr}(F\delta A\mathscr{A}+F\mathscr{A}\delta A+F\mathscr{A}D_A\mathscr{A})$$
$$-\frac{i}{16\pi^3}\delta\int_{S^3}\mathrm{tr}\left(\mathscr{A}\left(AF+FA-\frac{1}{2}A^3\right)\right), \tag{5.4}$$

and the Jacobi identity gives the "curvature" three-form

$$[E_X,[E_Y,E_Z]]+(\text{perm.})$$
$$=\delta\Omega^2(S^3)=Q^3(S^3)$$
$$=-\frac{i}{48\pi^3}\int_{S^3}\mathrm{tr}(\delta A\delta A\delta A)$$
$$-\frac{i}{48\pi^3}\int_{S^3}\mathrm{tr}(F\delta A\mathscr{A}+F\mathscr{A}\delta A+F\mathscr{A}D_A\mathscr{A}). \tag{5.5}$$

Note that the above anomalous terms in the commutation relation and the Jacobi identity differ from ones given by Niemi and Semenoff in Ref. 19. Our results reduce to theirs for $\mathscr{A}=0$.

Since the Jacobi identity fails, the covariant translations on $\mathfrak{A}^3$ are not associative and cannot form a Lie group.[25] However, since $\delta Q^3(S^3)=0$, the electric field trivially satisfies the algebra identity given by the present authors[26]

$$[E_X,[E_Y,[E_Z,E_W]]]+(\text{perm.})=\delta Q^3(S^3)=0. \tag{5.6}$$

As pointed out in Ref. 26, they do not form the so-called Malcev identity.[27]

It remains to examine the global properties of the $Q^3(S^3)$ and of the $\Omega^2(S^3)$. To this end, we integrate $Q^3(S^3)$ over the three-dimensional disk Δ^3 in $\mathfrak{A}^3$. Select Δ^3 so that its boundary $\partial\Delta^3=\Gamma^2$ is a two-dimensional sphere in $\mathscr{G}^3$, and its projection onto $\mathfrak{A}^3/\mathscr{G}$ is also a two-dimensional sphere. Then, from Eq. (5.3),

$$\int_{\Delta^3}Q^3(S^3)=\int_{\Delta^3}\delta\Omega^2(S^3)=\int_{\partial\Delta^3}\Omega^2(S^3)=\int_{\Gamma^2}\Omega^2(S^3)=\int_{\Gamma^2}\check{\Omega}^2(S^3)=\int_{\Gamma^2}\int_{S^3}\check{\omega}_3^2$$
$$=\int_{\Gamma^2_+}\int_{S^3}\check{\omega}_3^2-\int_{\Gamma^2_-}\int_{S^3}\check{\omega}_3^2=\int_{\Gamma^1}\int_{D^4_+}\check{\omega}_4^1-\int_{\Gamma^1}\int_{D^4_-}\check{\omega}_4^1=\int_{\Gamma^1}\int_{S^4}\check{\omega}_4^1$$
$$=\int_{\Gamma^1_+}\int_{S^4}\check{\omega}_4^1-\int_{\Gamma^1_-}\int_{S^4}\check{\omega}_4^1=\int_{\Gamma^0}\int_{D^5_+}\check{\omega}_5^0-\int_{\Gamma^0}\int_{D^5_-}\check{\omega}_5^0=\int_{\Gamma^0}\int_{S^5}\check{\omega}_5^0=Z, \tag{5.7}$$

which means that $\pi^3(\mathfrak{A}^3/\mathscr{G}^3)=\pi^2(\mathscr{G}^3)=Z$. Thus we show that there exists a noncontractible three-dimensional sphere in $\mathfrak{A}^3/\mathscr{G}^3$.

VI. GENERALIZATION TO A NONTRIVIAL PRINCIPAL BUNDLE

When the principal bundle $P(M,G)$ is nontrivial, the theory is slightly complicated. We choose a fixed background connection[15,28] form $\mathring{A}$ on P and extend it to $P\times\mathfrak{A}$. We shall not transform $\mathring{A}$, i.e., $\delta\mathring{A}=0=\delta_h\mathring{A}=0=\delta_v\mathring{A}$. Therefore the extension of $\mathring{A}$ from P to $P\times\mathfrak{A}$ is still $\mathring{A}$. The corresponding curvature form is

$$\mathring{F}=d\mathring{A}+\tfrac{1}{2}[\mathring{A},\mathring{A}]. \tag{6.1}$$

Equation (2.24) used in Sec. II is replaced by

$$P_{2n}(\mathscr{F}^n)-P_{2n}(\mathring{F}^n)=(d+\delta)\omega_{2n-1}(A+\mathscr{A},\mathring{A}). \tag{6.2}$$

This can be shown easily as follows: Let $\tilde{A}_t=t(A+\mathscr{A})+(1-t)\mathring{A}$. Then

$$\tilde{F}_t=(d+\delta)\tilde{A}_t+\tfrac{1}{2}[\tilde{A}_t,\tilde{A}_t], \tag{6.3}$$

$$\frac{\partial\tilde{F}_t}{\partial t}=(d+\delta)\frac{\partial\tilde{A}_t}{\partial t}+\left[A_t,\frac{\partial\tilde{A}_t}{\partial t}\right]\equiv\tilde{D}_t\frac{\partial\tilde{A}_t}{\partial t}. \tag{6.4}$$

The Bianchi identity is

$$\tilde{D}_t\tilde{F}_t\equiv(d+\delta)\tilde{F}_t+[\tilde{A}_t,\tilde{F}_t]=0. \tag{6.5}$$

Therefore

$$\frac{\partial}{\partial t}P_{2n}(\tilde{F}_t^n)=nP_{2n}\left(\frac{\partial\tilde{F}_t}{\partial t},\tilde{F}_t^{n-1}\right)$$
$$=nP_{2n}\left(\tilde{D}_t\frac{\partial\tilde{A}_t}{\partial t},\tilde{F}_t^{n-1}\right)$$
$$=(d+\delta)nP_{2n}\left(\frac{\partial\tilde{A}_t}{\partial t},\tilde{F}_t^{n-1}\right)$$
$$=n(d+\delta)P_{2n}(A+\mathscr{A}-\mathring{A},\tilde{F}_t^{n-1}).$$

Integrating the above equation with respect to t from 0 to 1 gives

$$P_{2n}(\mathscr{F}^n)-P_{2n}(\mathring{F}^n)$$
$$=(d+\delta)n\int_0^1 dt\,P_{2n}(A+\mathscr{A}-\mathring{A},\tilde{F}_t^{n-1}). \tag{6.6a}$$

Thus

$$\omega_{2n-1}(A+\mathscr{A},\mathring{A})=n\int_0^1 dt\,P_{2n}(A+\mathscr{A}-\mathring{A},\tilde{F}_t^{n-1}). \tag{6.6b}$$

Integrating Eq. (6.2) over M_{2n-k} without boundary, we still have

$$Q^k(M_{2n-k})=\delta\Omega^{k-1}(M_{2n-k}). \tag{6.7}$$

Here

$$Q^k(M_{2n-k})=\int_{M_{2n-k}}P_{2n}(\mathscr{F}^n), \tag{6.8}$$

$$\Omega^{k-1}(M_{2n-k}) = \int_{M_{2n-k}} \omega_{2n-1}(A + \mathcal{A}, \mathring{A}). \tag{6.9}$$

Equation (6.2), when limited to fiber, becomes

$$P_{2n}(F^n) - P_{2n}(\mathring{F}^n) = (d + \delta_v)\omega_{2n-1}(A + v, \mathring{A}). \tag{6.10}$$

Using the expansion of $\omega_{2n-1}(A + v, \mathring{A})$ in v,

$$\omega_{2n-1}(A + v, \mathring{A}) = \sum_k \omega^k_{2n-k-1}(v; A, \mathring{A}), \tag{6.11}$$

we can easily show that

$$\begin{aligned} &P_{2n}(F^n) - P_{2n}(\mathring{F}^n) = d\omega^0_{2n-1}(v; A, \mathring{A}), \\ &\delta_v \omega_0^{2n-1}(v; A, \mathring{A}) = 0, \\ &\delta_v \omega^{k-1}_{2n-k}(v; A, \mathring{A}) = -d\omega^k_{2n-k-1}(v; A, \mathring{A}). \end{aligned} \tag{6.12}$$

We thus obtain the double-cohomological series in the nontrivial case.[28]

Note that all formulas so far written, together with the unchanged expressions in Sec. II, are global on $P(M,G)$ and that only for a trivial bundle one can choose $\mathring{A} = 0$ and recover the local formulas in Sec. II.

VII. CONCLUSION AND DISCUSSION

We have stressed the relation and difference between an arbitrary variation δ, and the horizontal δ_h and the vertical δ_v ones in connection space. By using the natural connection form on the bundle $P(M,G)$ and $\mathfrak{A}(\mathfrak{A}/\mathcal{G}, \mathcal{G})$ and by introducing integration over an arbitrary chain, the generalized finite double-cohomological series can be obtained. Thus the relation between these cohomologies, and the family index theorem can be made simple and obvious. When applying this formalism to analyze Abelian gauge structure inside non-Abelian gauge theory, we reproduce known results in Refs. 18 and 19, and also give some new expressions. The method discussed here has a few important advantages: First, it is very simple. Second, it exposes the mathematical origin of Abelian gauge structures in the sense that these structures can be analyzed by the method. Finally, it can easily be generalized to higher dimensions and to other theories such as gravitational and supersymmetric Yang–Mills theories.

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Large rectangular random matrices

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Models with a multiplet of field variables arranged into rectangular matrices, in the limit of infinite dimensions of the matrices, are studied. In zero-dimensional space (where the problem is a combinatorial one) a closed solution is given that improves the one previously known. In arbitrary space dimension a symmetry is described that connects rectangular models with vector models.

I. INTRODUCTION

Gaussian ensembles of large matrices with given symmetry group have been used for a long time to describe the fluctuations around the average distribution of highly excited energy levels of heavy nuclei.[1] As the measure in probability space is taken to be Gaussian, these ensembles may be said to be models of noninteracting matrices. More recently, in the study of a discrete formulation of a statistical mechanics for surfaces, ensembles of Hermitian matrices with a cubic interaction were studied.[2] An ensemble of two sets of matrices with quartic self-interaction and a quadratic coupling was shown to define an Ising model on a random lattice in a two-dimensional space.[3] All these models considered square matrices in the limit of infinite dimension. Some attempts are currently being made to relate the statistical mechanics of a randomly triangulated surface to a viable discretized string model.

Our main interest in evaluating matrix models in the large N limit is presently oriented to quantum field theory. We then use a language appropriate for it, even in Sec. II, where we limit ourselves to a zero-dimensional space-time and the quantum field theoretical model is merely a combinatorial problem. Field theoretical models with multicomponent field variables are of substantial interest in themselves as well as tools for nonperturbative calculations. The two most popular classes of models have the field variables arranged as vectors or square matrices, and the low-order invariants built with them provide for the Lagrangian. Models with fields arranged into rectangular matrices offer an obvious interpolation between the two classes and were recently studied.[4–7]

This paper continues the study of rectangular models. In Sec. II we define a model of interacting rectangular matrices of sides N_1, N_2 and solve it in the limit $N_1 \to \infty$ and $N_2 \to \infty$, with fixed ratio $L \equiv N_1/N_2$. We evaluate the Green's functions for the entire range of the dimensionless variable $-\infty < m^2/\sqrt{g} < \infty$; the present derivation is simpler than the one previously known, which is valid in a more restricted range.[4]

In Sec. III we describe an exact symmetry property of the planar Green's functions[6] of rectangular models with generic interaction, valid in any dimension of space-time, which gives the simple relation between "internal loop expansion" and "large N expansion" of vector models.

II. A ZERO-DIMENSIONAL MODEL

We consider the partition function for the model

$$Z = Z_0^{-1} \int [DM] \times \exp\left\{ -\mathrm{tr}\left[\frac{m^2}{2} M^T M + \frac{g}{N} M^T M M^T M \right] \right\}, \tag{1}$$

where M is a real $NL \times N$ matrix, M^T is its transpose, $L \geqslant 1$,

$$Z_0 \equiv \int [DM] \exp\left\{ -\mathrm{tr}\left[\frac{|m^2|}{2} M^T M \right] \right\}, \tag{2}$$

and

$$[DM] \equiv \prod_{\substack{i=1,\ldots,NL \\ j=1,\ldots,N}} dM_{ij}. \tag{3}$$

Because of the invariance of the Lagrangian under the symmetry group $O(NL) \times O(N)$, it is convenient to rewrite M in the canonical form $M = O_1 \Lambda O_2$ with $\Lambda_{ij} = \lambda_i \delta_{ij}$ for $1 \leqslant i, j \leqslant N$ and $\Lambda_{ij} = 0$ for $N < i \leqslant NL$, $1 \leqslant j \leqslant N$, $O_1 \in O(NL)$, $O_2 \in O(N)$. The action depends upon the N real variables λ_i, whereas the integration over the "angular variables" cancels because of the normalization of the partition function. As shown by Simonis[7] we may write

$$Z \sim \int \prod_{i=1}^{N} d\lambda_i |\lambda_i|^{(L-1)N} \prod_{1 \leqslant i < j \leqslant N} |\lambda_i^2 - \lambda_j^2| \times \exp\left[-\sum_k \left(\frac{m^2}{2} \lambda_k^2 + \frac{g}{N} \lambda_k^4 \right) \right]. \tag{4}$$

Here and in the following we neglect factors irrelevant to the evaluation of the Green's functions. In terms of the quadratic variables $t_i \equiv \lambda_i^2/N$, $i = 1,\ldots,N$, we obtain

$$Z \sim \int \left(\prod_{i=1}^{N} dt_i \right) \exp\left\{ -N \sum_i \left(\frac{m^2}{2} t_i + g t_i^2 - \frac{L - 1 - 1/N}{2} \log t_i - \frac{1}{N} \sum_{i<j} \log |t_i - t_j| \right) \right\}. \tag{5}$$

The large N limit is performed by the standard method[8] of introducing the continuous function $t(x)$ and looking for the saddle point:

$$Z \sim \int dt(x) \exp\left\{ -N^2 \int_0^1 dx \left[\frac{m^2}{2} t(x) + g t^2(x) - \frac{L-1}{2} \log t(x) - \frac{1}{2} \int_0^1 dy \log |t(x) - t(y)| \right] \right\}, \tag{6}$$

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$$\frac{m^2}{2}+2gt(x)-\frac{L-1}{2}\frac{1}{t(x)}=\oint_0^1 dy\frac{1}{t(x)-t(y)}. \tag{7}$$

We might have considered the model (1) with M being a complex matrix. Since the appropriate measure would then be[7]

$$[D\lambda]=\prod_{i=1}^{N} d\lambda_i\,|\lambda_i|^{2(L-1)N}\prod_{1\leqslant i<j\leqslant N}|\lambda_i^2-\lambda_j^2|^2, \tag{8}$$

one sees that the present model is reproduced after the replacements $m^2/2\to m^2$, $g\to 2g$. The saddle point equation (7) is rewritten, in the usual way, in terms of the density $u(t)\equiv dx/dt$

$$\frac{m^2}{2}+2gt-\frac{L-1}{2}\frac{1}{t}=\oint_l ds\frac{u(s)}{t-s}. \tag{9}$$

The requirement that the variable t should be non-negative leads us to invert Eq. (9) by choosing the path l to be the segment $[A,B]$ with $0\leqslant A\leqslant B$. We find

$$u(t)=\frac{2g}{\pi}\sqrt{(B-t)(t-A)}\left(t+\frac{A+B}{2}+\frac{m^2}{4g}\right)\frac{1}{t}, \tag{10}$$

where

$$(A+B)^2+\frac{(B-A)^2}{2}+\frac{m^2}{2g}(A+B)=\frac{L+1}{g}, \tag{11}$$

$$\sqrt{AB}\,[m^2+2g(A+B)]=L-1. \tag{12}$$

The even-order planar Green's functions are easily evaluated:

$$G_{2n}^{\rm pl}\equiv\lim_{N\to\infty}\frac{\langle \mathrm{tr}(M^TM)^n\rangle}{N^{n+1}}=\int_l dt\,t^n u(t). \tag{13}$$

The special case of square matrices ($L=1$) implies, by Eq. (12), either $A=0$ or $m^2+2g(A+B)=0$. The first choice immediately leads to the Saclay solution,[8] which holds for $m^2/\sqrt{g}\geqslant -4$. The latter choice gives

$$u(t)=(2g/\pi)\sqrt{(B-t)(t-A)}, \tag{14}$$

and the corresponding Green's functions are those of a Gaussian model with nonvanishing average.[9] In the truly rectangular case, $L>1$, the lower extremum A is strictly positive and the density $u(t)$ is non-negative for every real m^2 and positive g. We also verify that the system (11), (12) has a unique solution for A,B in the whole range of the parameters ($L>1, g>0, m^2$ real) and that the solution is continuous as a function of the parameters, thus suggesting the existence of a unique phase for this model. The density may be written

$$u(t)=\frac{1}{\pi}\sqrt{(B-t)(t-A)}\left(2g+\frac{1}{2t}\frac{L-1}{\sqrt{AB}}\right). \tag{15}$$

One trivially finds

$$G_{2n}=2gI_n+[(L-1)/2\sqrt{AB}\,]I_{n-1},\quad n\geqslant 1,\quad L>1, \tag{16}$$

with

$$I_n\equiv[(B-A)^2/8]A^n\,{}_2F_1(-n,\tfrac{3}{2};3;1-B/A), \tag{17}$$

in particular,

$$G_2=[(B-A)^2/16][m^2+4g(A+B)], \tag{18}$$

$$G_4=\frac{(B-A)^2}{16}\left[\frac{m^2}{2}(A+B)-gAB+\frac{9}{4}g(A+B)^2\right]. \tag{19}$$

We note the special case $L\geqslant 1$, $m^2>0$, $g=0$. The system (11), (12) is then solved by

$$A=[(\sqrt{L}-1)/m]^2,\quad B=[(\sqrt{L}+1)/m]^2 \tag{20}$$

and one has

$$\begin{aligned}G_{2n}&=\frac{m^2}{\pi}\int_{\sqrt{A}}^{\sqrt{B}}dx\,x^{2n}\frac{\sqrt{(B-x^2)(x^2-A)}}{x}\\&=\frac{L(\sqrt{L}-1)^{2n-2}}{m^{2n}}\\&\quad\times{}_2F_1\left(-n+1,\frac{3}{2};3;\frac{-4\sqrt{L}}{(\sqrt{L}-1)^2}\right).\end{aligned} \tag{21}$$

By comparing Eq. (21) with the square matrix case ($L=1$),

$$G_{2n}=\frac{m^2}{\pi}\int_0^{2/m}dx\,x^{2n}\sqrt{\frac{4}{m^2}-x^2}=\frac{(2n)!}{n!(n+1)!}\frac{1}{m^{2n}}, \tag{22}$$

we see that the density

$$u(x)=\begin{cases}\dfrac{m^2}{\pi}\dfrac{\sqrt{(B-x^2)(x^2-A)}}{x}, & \sqrt{A}\leqslant x\leqslant\sqrt{B},\\ 0, & \text{elsewhere},\end{cases} \tag{23}$$

is the generalization of the Wigner semicircle distribution,[1] for the case of rectangular matrices.

The rectangular case with $0<L<1$ is obtained from Eqs. (10)–(13) by exploiting a symmetry property that holds in any dimension of space-time and which we now discuss.

III. SYMMETRY OF PLANAR RECTANGULAR GREEN'S FUNCTIONS

In Euclidean $\mathbb{R}^d$ space, we consider the Lagrangian density

$$\begin{aligned}\mathscr{L}(M(x))=\mathrm{tr}[&\partial_\mu M^T(x)\,\partial_\mu M(x)\\&+(m^2/2)M^T(x)M(x)\\&+gM^T(x)M(x)M^T(x)M(x)]\end{aligned} \tag{24}$$

and the set of singlet Green's functions

$$\begin{aligned}&F_{2n}(x_1,x_2,\ldots,x_{2n};m^2,g,NL,N)\\&=\int[DM(x)]\,\mathrm{tr}(M^T(x_1)M(x_2)\cdots M(x_{2n}))\\&\quad\times\exp\left(-\int d^dx\,\mathscr{L}(M(x))\right)\left[\int[DM(x)]\right.\\&\quad\left.\times\exp\left(-\int d^dx\,\mathscr{L}(M(x))\right)\right]^{-1}.\end{aligned} \tag{25}$$

The exchange $NL\leftrightarrow L$ amounts to the exchange $M^T(x)\leftrightarrow M(x)$, which leaves the action and the measure invariant. Then

$$F_{2n}(x_1,x_2,\ldots,x_{2n};m^2,g,NL,N) = F_{2n}(x_2,x_3,\ldots,x_1;m^2,g,N,NL)\,. \tag{26}$$

These Green's functions have a nontrivial large N limit, apart from the overall factor N^{n+1}, provided that g is replaced by g/Nk, where the parameter k is independent of N. That is,

$$\lim_{N\to\infty} N^{-(n+1)}F_{2n}(x_1,x_2,\ldots,x_{2n};m^2,g/Nk,NL,N) = G^{\rm pl}_{2n}(x_1,x_2,\ldots,x_{2n};m^2,g/k,L)\,. \tag{27}$$

The symmetry property (26) then implies

$$G^{\rm pl}_{2n}(x_1,x_2,\ldots,x_{2n};g/k,L) = L^{n+1}G^{\rm pl}_{2n}(x_2,x_3,\ldots,x_1;g^L/k,1/L) = L^{n+1}G^{\rm pl}_{2n}(x_1,x_2,\ldots,x_{2n};gL/k,1/L)\,, \tag{28}$$

where, in the last equality, we exploited the invariance of planar Green's functions under cyclic permutations.

The most symmetric choice for the constant k follows from the geometrical mean of the numbers of rows and columns, that is, $k=\sqrt{L}$ and it leaves the coupling constant $\tilde{g}\equiv g/\sqrt{L}$ in the $G^{\rm pl}_{2n}$ unchanged under the symmetry:

$$G^{\rm pl}_{2n}(x_1,x_2,\ldots,x_{2n};\tilde{g},L) = L^{n+1}G^{\rm pl}_{2n}(x_1,x_2,\ldots,x_{2n};\tilde{g},1/L)\,. \tag{29}$$

We note that by this choice for the parameter k the obvious invariance of the theory under the exchange between rows and columns, Eq. (26), is represented in the planar limit in the most natural way, Eq. (29).

The model with rectangular matrices interpolates in some way between models with square matrices and vector models. However, the choice $k=\sqrt{L}$ is such that the $G^{\rm pl}_{2n}(x_1,x_2,\ldots,x_{2n};g/\sqrt{L},L)$ have no nontrivial expansions at fixed g either around $L=0$ or at $L=\infty$. To be more specific, we consider the $O(L)$ symmetric Lagrangian model with a vector of L real field components Φ_i, $i=1,\ldots,L$, with the quartic interaction

$$\mathscr{L}_{\rm int} = g[\Phi(x)\cdot\Phi(x)]^2\,, \tag{30}$$

the set of Green's functions

$$\mathscr{G}_{2n}(x_1,x_2,\ldots,x_{2n};g,L) \equiv \left\langle \prod_{i=1}^{2n-1} \Phi(x_i)\cdot\Phi(x_{i+1}) \right\rangle, \tag{31}$$

and the usual large L expansion

$$\mathscr{G}_{2n}\left(x_1,\ldots,x_{2n};\frac{g}{L},L\right) = L^n\sum_{j=0}^{\infty}\left(\frac{1}{L}\right)^j \mathscr{G}_{2n,j}(x_1,\ldots,x_{2n};g)\,. \tag{32}$$

The planar (that is, $N=\infty$) rectangular Green's functions $G^{\rm pl}_{2n}(x_1,\ldots,x_{2n};g/k,L)$ have a nontrivial large L expansion, provided $k=L$:

$$G^{\rm pl}_{2n}\left(x_1,\ldots,x_{2n};\frac{g}{L},L\right) = L^n\sum_{j=0}^{\infty}\left(\frac{1}{L}\right)^j G^{\rm pl}_{2n,j}(x_1,\ldots,x_{2n};g)\,. \tag{33}$$

At arbitrary order in perturbation theory it is easy to check that $G^{\rm pl}_{2n,j}(x_1,\ldots,x_{2n};g)$ is the planar part of the graphs that contribute to $\mathscr{G}_{2n,j}(x_1,\ldots,x_{2n};g)$. Since in the first two orders in the large L expansion of the vector model, Eq. (32), only planar graphs contribute, it follows that

$$\mathscr{G}_{2n,j}(x_1,\ldots,x_{2n};g) = G^{\rm pl}_{2n,j}(x_1,\ldots,x_{2n};g) \quad \text{for } j=0,1\,. \tag{34}$$

From the symmetry property, Eq. (28), one obtains some interesting consequences that hold for the generic vector model in arbitrary space-time dimension. Consider, for instance, the $\mathscr{L}_{\rm int}$ given in Eq. (30). One may introduce an auxiliary field (random field) to transform the original quartic interaction into a cubic one (with imaginary coupling constant). In this case, the evaluation of Green's functions, Eq. (31), in the expansion in the number of loops of the original vector field (which we called internal loop expansion[4,5]) is obviously the Taylor expansion around $L=0$ of Eq. (31):

$$\mathscr{G}_{2n}(x_1,\ldots,x_{2n};g,L) = \sum_{j=0}^{\infty} L^j g_{2n,j}(x_1,x_2,\ldots,x_{2n};g)\,. \tag{35}$$

The previous discussion for rectangular models implies that the planar part of $g_{2n,j}(x_1,\ldots,x_{2n};g)$ equals the planar part of $\mathscr{G}_{2n,j}(x_1,\ldots,x_{2n};g)$ for every j and n.

The closed solution of the large rectangular matrix problem in zero dimensions, derived in Sec. II, allows us to verify the symmetry, Eq. (28), in a straightforward way. Indeed, the solutions gA and gB of the system (10), (11), depend on g and L only through the two combinations $u_1\equiv g(L+1)$ and $u_2\equiv g|L-1|$, which are invariant under the symmetry.

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Waves, bifurcations, and solitons in a model with sixfold symmetry

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The traveling-wave solutions of a model Lagrangian density for a complex-valued scalar field with possible application to charge density waves in systems with sixfold symmetry are explored by means of the slow-fluctuation technique. There are five main wave types separated by three bifurcations with respect to integration constants. In addition, there are several classes of degenerate waves, including some with purely harmonic, stable, straight-line or circular motions of the amplitude vector. Beyond the range of the slow-fluctuation approximation there are several unstable soliton solutions, three of which have unexpectedly curved paths of the amplitude vector.

I. INTRODUCTION

We present here an overview of all traveling-wave solutions for the complex-valued scalar field $\psi(x,t) = u(x,t) \times \exp[i\phi(x,t)]$ having the Lagrangian density

$$\mathscr{L} = \tfrac{1}{2}|\psi_t|^2 - \tfrac{1}{2}|\psi_x|^2 + \tfrac{1}{2}A|\psi|^2 - \tfrac{1}{4}B|\psi|^4 - D|\psi|^N(1-\cos N\phi) \qquad (1.1)$$

with $N = 6$, where A, B, and D are positive constants. This model has possible applications in the theory of charge density waves in crystals where the symmetry-breaking last term of (1.1) can approximate the effects of commensurability pinning of lattice period and wave period.[1,2]

We have previously treated[2] the case $N = 4$ in the slow-fluctuation approximation,[3-7] which for this system remains numerically accurate up to moderately large amplitudes over a hundred periods or so. Three main wave types were found. They are separated by two bifurcations, one with respect to a coupling strength $\lambda = 1 + 16D/B$, the other with respect to an integration constant c_1 equivalent to an energy. There are also various constant-amplitude (c-a) waves, and beyond the limits of validity of the approximation there are several obvious solitons that had been noticed before.[8]

The case $N = 6$, with sixfold instead of fourfold symmetry, is far more involved. There are five main wave types, and an additional bifurcation with respect to an integration constant α. There are again various c-a waves and obvious solitons. Furthermore, if we extrapolate our classification of waves in a qualitative way beyond its quantitative validity, we are led to conjecture certain unexpected soliton solutions, and indeed, some numerical experimentation confirmed the existence of three such curious solitons, only one of which has a certain parallel in a soliton discovered previously in the $N = 2$ system.[9]

Given the complexity of the case, we take license to describe our main results by means of graphs and running commentary without detailed derivations. However, we specify enough close links with the exposition in Ref. 2 to enable the reader to supply all derivations easily, albeit with considerable tedium. Readers who seek access to the results at the expense of skipping these links altogether will find it helpful occasionally to turn forward to Figs. 7 and 8 which display the classification of all waves (of moderate amplitude) from different points of view.

The numerical accuracy of our approximation was checked by means of a large sample of test cases calculated at the system parameter values $\lambda' = \frac{1}{4}$ and $\lambda' = 2$. The results were virtually the same as for the $N = 4$ system, which we have discussed[2] in detail: in most cases, graphs of the approximate and the exact solution are indistinguishable over some 100 wave periods, provided the wave amplitude does not exceed one-fourth of the maximal finite value (i.e., one-fourth of the distance from the origin to the saddle point in Fig. 1 below). For initial conditions near unstable waves, the approximate solutions were often less accurate, as can be expected. Still, as a qualitative predictor of wave types and bifurcations the slow-fluctuation approach is fully effective even near these dynamical instabilities.

II. TRAVELING WAVES

Traveling, undistorted waves are functions of the variable $s = (x - vt)(1 - v^2)^{-1/2}$ only. When we introduce this quasitime in (1.1), and also scale the variables as in Ref. 2 in order to hide numerical coefficients, the Lagrangian density becomes a Lagrangian function for the motion of a fictitious unit point mass in the potential

$$V(\xi,\eta) = \tfrac{1}{2}(\xi^2+\eta^2) - \tfrac{1}{4}(\xi^2+\eta^2)^2 - \lambda'(3\xi^2-\eta^2)^2\eta^2, \quad \lambda' = 2AD/B^2, \qquad (2.1)$$

where ξ and η are the (scaled) real and imaginary parts of the wave function $\psi(s)$.

The potential has sixfold symmetry. From a central basin three ridges issue along the directions $\eta = 0$ and $\eta = \pm\xi\sqrt{3}$; they lead to six hilltops at unit distance from the origin. Between the hills lie six saddles along the directions $\xi = 0$ and $\eta = \pm\xi/\sqrt{3}$. Beyond hills and saddles, the potential falls off to negative values everywhere. Figure 1 shows contour maps for $\lambda' = \frac{1}{4}$ and $\lambda' = 2$.

The moving point mass represents the end point of the

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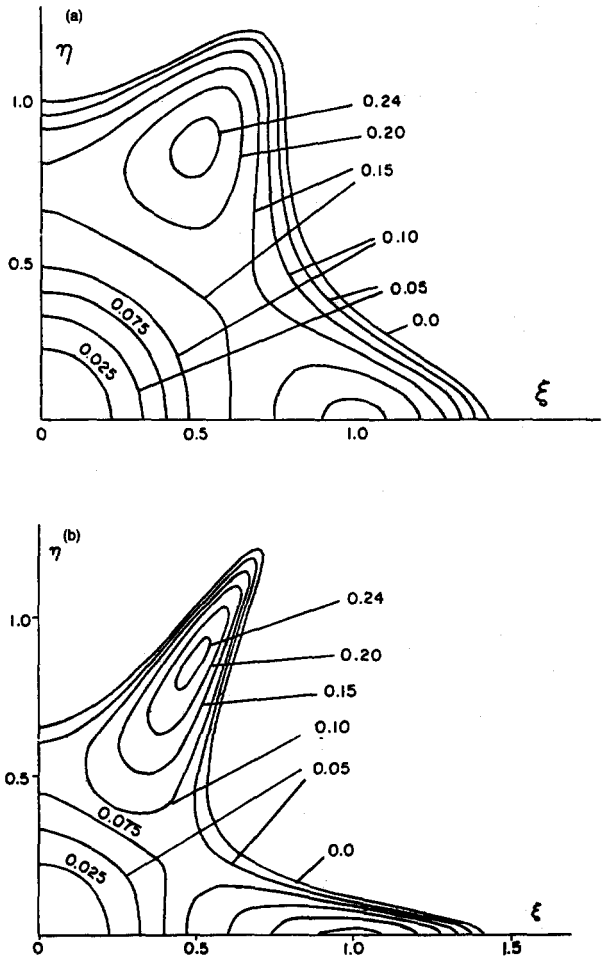

FIG. 1. Contour maps of the potential (2.1) in the first quadrant. To obtain the complete figure resembling a six-star, adjoin mirror images on the left, and below the ξ axis: (a) $\lambda' = \frac{1}{4}$, (b) $\lambda' = 2$.

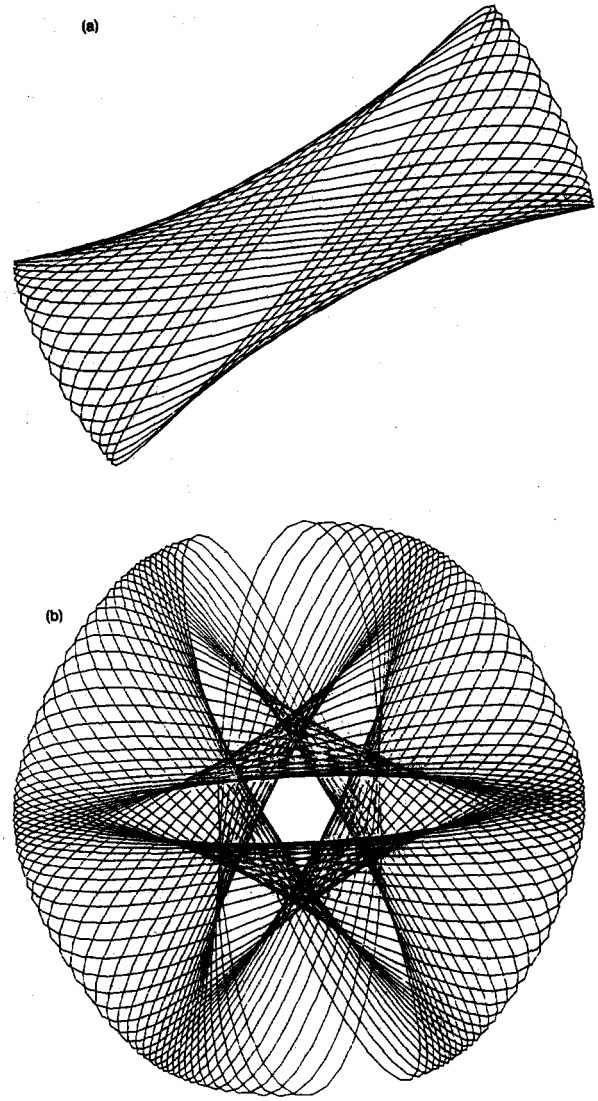

FIG. 2. Two representative orbits in the potential of Fig. 1(a) with $\lambda' = \frac{1}{4}$, and below the α bifurcation. Scales enlarged over Fig. 1. (a) Valley libration corresponding to even–even modulation between R_4 and R_6 in Fig. 5(a) or 5(b). Set up from R_6 by release from rest at $\xi = 0.3768$ and $\eta = 0.0447$; $\alpha = 0.072$, hence $\lambda'\alpha = 0.018 < \frac{1}{3}$. (b) "Narrow" precession corresponding to odd–odd modulation between R_1 and R_3 in Fig. 5(c). Set up from R_1 by transverse launch at $\xi = 0.1020$ and $\eta = 0$ with $\dot{\eta} = -0.3481$; $\alpha = 0.0649$, hence $\lambda'\alpha = 0.016 < \frac{1}{3}$.

amplitude vector of a transverse ψ wave as seen by an observer at a stationary place x who looks along the propagation vector. At infinitesimal amplitudes the motion in the central basin will be purely harmonic, with both component frequencies being equal, $\omega_\xi = \omega_\eta = 1$, as seen from the leading term in the potential (2.1); thus, the orbit is elliptical. At finite amplitudes, precessions and librations of the orbit set in. The approximation to be developed below shows that there are five motion types possible (plus degenerate or special cases). We display representatives of these right now in Figs. 2 and 3, as obtained by numerical integration of the exact equations of motion.

Figure 2 shows two typical motions in the potential of Fig. 1(a). In Fig. 2(a) we see a "valley libration," a rather obvious hence-and-forth motion in the valley at 30° to the ξ axis. It resembles an almost linear polarization which goes to almost elliptical and back as the polarization axes librate about the 30° line. Figure 2(b) shows what we call a "narrow precession;" the motion remains nearly elliptical at all times, although with appreciably changing width, and it steadily precesses.

Figure 3 shows three typical motions in the potential of Fig. 1(b). In Fig. 3(a) we have a valley libration with rather more shape change than the one in Fig. 2(a). Figure 3(b) shows a precessing oval with relatively little change of shape; since the oval remains broad we call this precession "wide." Figure 3(c) brings something entirely different; a "ridge libration," with the mass point always deflected towards the ridges so strongly that it moves towards a hilltop rather than a saddle.

III. THE SLOW-FLUCTUATION APPROXIMATION

This section is closely aligned with Ref. 2, and all variables and functions have the same meaning.

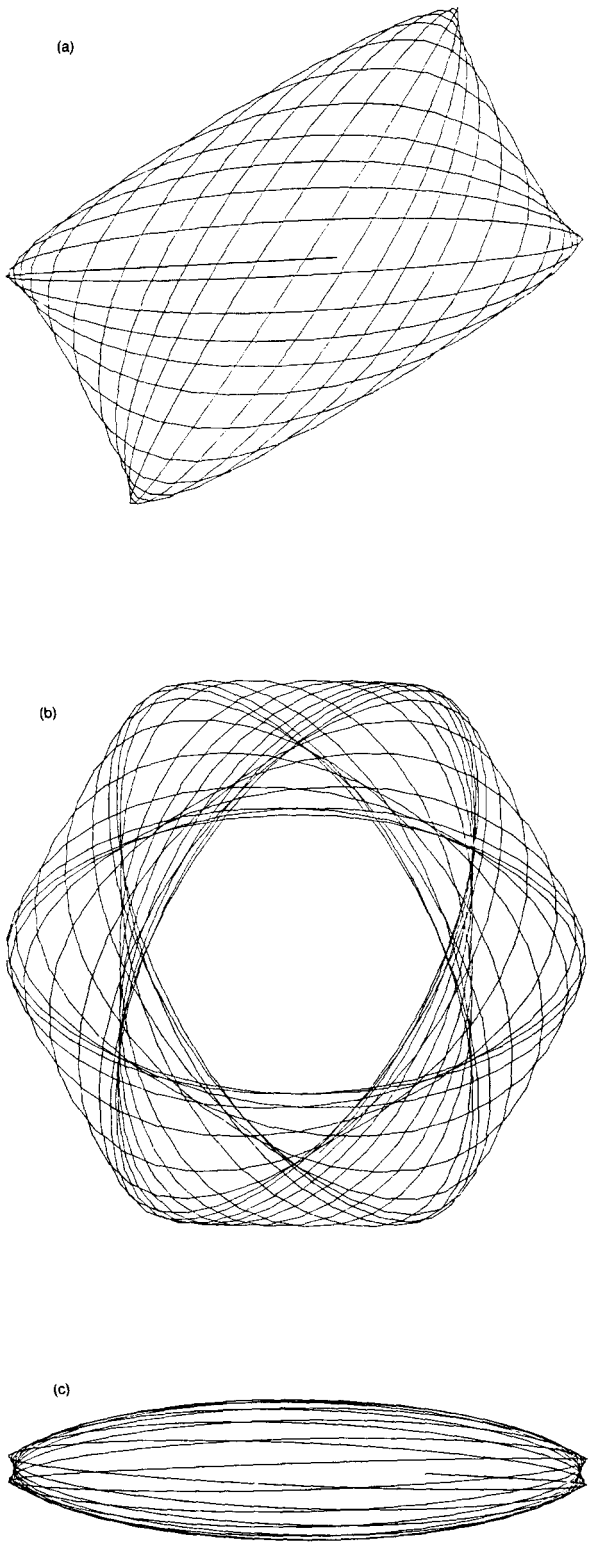

FIG. 3. Three representative orbits in the potential of Fig. 1(b) with $\lambda' = 2$. Scales enlarged over Fig. 1. All three are above the α bifurcation, with the same $\alpha = 0.077$, hence $\lambda'\alpha = 0.154 > \frac{1}{9}$. (a) Valley libration corresponding to even–even modulation between R_4 and R_6 in Fig. 6(a). Set up from R_4 by release from rest at $\xi = 0.2191$ and $\eta = 0.3256$. (b) "Wide" precession corresponding to odd–odd modulation between R_1 and R_3 in Fig. 6(b). Set up from R_1 by transverse launch at $\xi = 0.2280$ and $\eta = 0$ with $\dot{\eta} = -0.3194$. (c) Ridge libration corresponding to odd–even modulation between R_5 and R_6 in Fig. 6(b). Set up from R_6 by release from rest at $\xi = 0.3920$ and $\eta = 0.0173$.

In terms of the canonical amplitudes and phases $\bar{p}_j, \bar{q}_j$ (sometimes called "action-angle variables") the approximate but integrable slow-fluctuation Hamiltonian for the potential (2.1) is found to be

$$\begin{aligned}\overline{S} = {} & \bar{p}_1 + \bar{p}_2 - \tfrac{3}{8}\bar{p}_1^2 - \tfrac{1}{2}\bar{p}_1\bar{p}_2 - \tfrac{3}{8}\bar{p}_2^2 \\ & - \tfrac{27}{2}\lambda'\bar{p}_1^2\bar{p}_2 + 9\lambda'\bar{p}_1\bar{p}_2^2 - \tfrac{5}{2}\lambda'\bar{p}_2^3 \\ & + [\,-\tfrac{1}{4}\bar{p}_1\bar{p}_2 - 9\lambda'\bar{p}_1^2\bar{p}_2 + 6\lambda'\bar{p}_1\bar{p}_2^2\,] \\ & \times\cos(2\bar{q}_1 - 2\bar{q}_2). \end{aligned} \tag{3.1}$$

The integration procedure by means of the first integrals

$$\bar{p}_1 + \bar{p}_2 = \alpha, \quad \overline{S} = E, \tag{3.2}$$

and using the abbreviation

$$c_1 = E - \alpha + \tfrac{3}{8}\alpha^2 + \tfrac{5}{2}\lambda'\alpha^3, \tag{3.3}$$

yields the differential equation for the ξ amplitude,

$$\begin{aligned}\dot{\bar{p}}_1^2 = {} & f(\bar{p}_1) \\ = {} & -(2\overline{P} - 2\overline{F})(2\overline{P} + 2\overline{F}), \end{aligned} \tag{3.4}$$

$$\overline{F}(\bar{p}_1;\alpha) = \bar{p}_1(\alpha - \bar{p}_1)(6\lambda'\alpha - 15\lambda'\bar{p}_1 - \tfrac{1}{4}), \tag{3.5}$$

$$\begin{aligned}\overline{P}(\bar{p}_1;\alpha) = {} & c_1 - 25\lambda'\bar{p}_1^3 + (39\lambda'\alpha + \tfrac{1}{4})\bar{p}_1^2 \\ & - (\tfrac{33}{2}\lambda'\alpha^2 + \tfrac{1}{4}\alpha)\bar{p}_1. \end{aligned} \tag{3.6}$$

The polynomial $f(\bar{p}_1)$ is seen to be of the sixth degree, so that Eq. (3.4) leads to hyperelliptic integrals. General analytic solutions as in the case $N = 4$ are not available,[2] but an adequate discussion of the all-important roots of $f(\bar{p}_1)$ is still possible.

The astonishing complexity of the Hamiltonian (3.1), and of the equivalent Eq. (3.4), must be attributed in part to the use of coordinates suited for fourfold symmetries to describe a system with sixfold symmetry. However, there is intrinsic complexity as well. We mention in passing that for $N > 6$ in (1.1), several slowly fluctuating terms in the Hamiltonian arise beside the one with phase $2\bar{q}_1 - 2\bar{q}_2$; e.g., for $N = 8$ there is also one term with $4\bar{q}_1 - 4\bar{q}_2$. Thus, the higher N, the more complex the effects of the nonlinear coupling. An attempt to reduce these symmetry and nonlinearity complications by the use of other coordinates, say of plane polar coordinates, would only substitute complications of other types: at infinitesimal amplitudes we would no more be dealing with normal modes, the all-important conservation law $\bar{p}_1 + \bar{p}_2 = \alpha$ would take a much less simple form, and all discussions of orbital stability would become much more involved. Thus we prefer to put up with the complications in rectangular coordinates rather than lose so many theoretical tools.[3–6]

An attentive referee remarks that amongst workers in Hamiltonian mechanics our approximation would be called "first-order averaging," and goes on to ask: since it is well known[10] that first-order averaging of sixth-order terms should be accompanied by second-order averaging of fourth-order terms, why would we not include corresponding terms in our $\overline{S}$? The answer is starkly pragmatic: our $\overline{S}$ yields good results, as specified above. Here as in previous cases[2,7] we rest our claims for the usefulness of the method, and our justification for its lengthy theoretical development,[3–6] solely on its remarkable numerical accuracy. Of course, we are

only interested in accuracy over a hundred periods or so,[7] not in long-term behavior, ergodic properties, approach to chaos, or the like. Even so, we have enough insights of high generality to offer; cf. the stability and bifurcation results in Refs. 2, 4, 6, and 7, and those presented in Figs. 7 and 8 below.

IV. THE ROOTS OF $f(\bar{p}_1)$

The roots of $f(\bar{p}_1)$ are called even or odd according as they are roots of the first or of the second factor on the right of Eq. (3.4), respectively. We denote them by $R_{2,4,6}$ and $R_{1,3,5}$, respectively, and order them by $R_2 \leqslant R_4 \leqslant R_6$ and $R_1 \leqslant R_3 \leqslant R_5$ if real. On root parity in general, see Refs. 2 and 5.

From the explicit expressions (3.5) and (3.6) it follows that the roots satisfy

$$\bar{p}_1 = R_{2,4,6}: \ \tfrac{5}{2}\bar{p}_1(4\bar{p}_1 - 3\alpha)^2 = c_1/\lambda', \tag{4.1}$$

$$\bar{p}_1 = R_{1,3,5}: \ \tfrac{1}{2}\bar{p}_1[20\bar{p}_1^2 - (36\alpha + 1/\lambda')\bar{p}_1 + 21\alpha^2 + \alpha/\lambda'] = c_1/\lambda'. \tag{4.2}$$

At given λ', α, and c_1, these equations are easily solved graphically by curves representing the left-hand sides intersecting a horizontal line at the level c_1/λ'. Figure 4 gives an overview of these curves over the interval $[0,\alpha]$ where the physically relevant roots are located. The resulting root configurations are easy to understand graphically, but their algebraic discussion is tedious. A forward glance at Figs. 5 and 6 may help to avoid confusion.

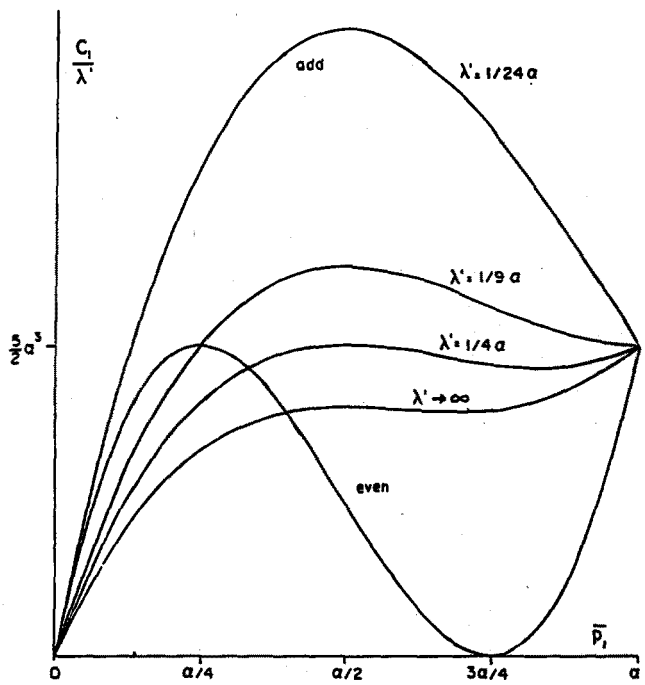

FIG. 4. Graphical determination of the physically relevant roots of $f(\bar{p}_1)$ at given λ', α, and c_1 (to scale). The even curves do not depend on the system parameter λ', see Eq. (4.1), but the odd ones depend on λ' in a varying way. Hence there is one even curve for given α and c_1, but an entire family of odd curves depending on λ', four of which have been drawn for significant values of λ'. The roots are now obtained at the intersection(s) of any one of these curves with a horizontal at the height c_1/λ'.

Signal importance attaches to any confluence of two or more roots, i.e., to multiple roots. Double roots of definite parity correspond to extrema of the curves.

Two even second-order roots can exist: $R_4 = R_6 = 3\alpha/4$ occurs at $c_1 = 0$, and $R_2 = R_4 = \alpha/4$ occurs at

$$c_1 = c_{1,\text{even}}^* = 5\lambda'\alpha^3/2. \tag{4.3}$$

Both are conspicuous in Fig. 4.

Two odd second-order roots can exist: $R_3 = R_5 = 7\alpha/10 + 1/30\lambda'$ occurs at

$$c_1 = c_{1,\text{odd}}^* = (\lambda'\alpha - \tfrac{1}{24})[49(\lambda'\alpha)^2 + \tfrac{14}{3}\lambda'\alpha + \tfrac{1}{8}]/(5\lambda')^2, \tag{4.4}$$

but for sufficiently small $\lambda'\alpha$ this root will lie beyond $\bar{p}_1 = \alpha$, as seen from Fig. 4; second, $R_1 = R_3 = \frac{1}{2}\alpha$ always occurs at

$$c_1 = c_{1,\text{odd}}^{**} = \tfrac{1}{8}\alpha^2 + 2\lambda'\alpha^3. \tag{4.5}$$

Multiple roots which are both even and odd are called skew and require an intersection of the even curve with an odd curve. When

$$\alpha = \alpha^* = 1/9\lambda', \tag{4.6}$$

it is seen from Fig. 4 that there are two such intersections, that both involve an extremum, and that both lie at the same height $c_1/\lambda' = 5\alpha^3/2$. Hence at $\alpha = \alpha^*$ there are two skew triple roots: $R_1 = R_2 = R_4 = \alpha/4$ and $R_3 = R_5 = R_6 = \alpha$, and furthermore these occur jointly for $c_1 = c_{1,\text{even}}^* = c_{1,\text{odd}}^*$.

Two skew second-order roots are found at the end points of $[0,\alpha]$. Here $R_1 = R_2 = 0$ occurs at $c_1 = 0$ (and coexists with the even $R_4 = R_6$). Second, such a root lies at α, but the confluence is $R_3 = R_6$ if $\alpha < \alpha^*$ and $R_5 = R_6$ if $\alpha > \alpha^*$ (with the triple $R_3 = R_5 = R_6$ in between at $\alpha = \alpha^*$, when the other triple root happens to coexist as well).

Another skew second-order root lies inside the interval $[0,\alpha]$, provided $\lambda_1\alpha > 1/24$; it is seen from Fig. 4 that at the critical value $\lambda' = 1/24\alpha$ the odd curve just osculates the even one at the origin. The required curve intersection is found at the position $\Gamma = 2\alpha/5 - 1/60\lambda'$; the confluence is $R_1 = R_2$ if $\alpha < \alpha^*$ and $R_1 = R_4$ if $\alpha > \alpha^*$ (with the triple $R_1 = R_2 = R_4$ in between at $\alpha = \alpha^*$, when the other triple root happens to coexist as well). As can just be discerned in Fig. 4, this skew root happens to occur exactly at $c_1 = c_{1,\text{odd}}^*$ so that it always coexists with the odd $R_3 = R_5$; now it also becomes clear that the latter lies inside $[0,\alpha]$ only if $\alpha > \alpha^*$.

The values α^*, $c_{1,\text{even}}^*$ and $c_{1,\text{odd}}^*$ (and in a trivial way also $c_1 = 0$ and $c_{1,\text{odd}}^{**}$) are bifurcation values demarcating significant changes in the configuration of the roots of $f(\bar{p}_1)$ which carry over into significant changes of the orbit in the potential well. As will be shown below, the conspicuous, simultaneous occurrence of multiple roots merely reflects the symmetry of the potential well, which allows for several orbits of different orientations at the same λ', α, and c_1.

V. THE CONFIGURATIONS OF $f(\bar{p}_1)$

Since the coefficient of $\bar{p}_1^6$ in $f(\bar{p}_1)$ is negative, see Eq. (3.4), a qualitative graph of $f(\bar{p}_1)$ can be sketched at once when the locations of its real roots are known. They are best deduced from Fig. 4 by the following procedure which

emerges clearly from the algebraic classifications in the preceding section, and can also be justified in a very general way.[6] At a given system parameter λ', first select a value of the integration constant α; then vary the other constant c_1 by shifting a horizontal up and down in Fig. 4, and watch the resultant movement of the intersections. The corresponding configurations of $f(\bar{p}_1)$ at the more important stages of development are depicted in Figs. 5 and 6. Because of the existence of the bifurcation value at $\alpha^* = 1/9\lambda'$, we must go through this procedure twice at least, for a value of α below and another above α^*; the two cases are illustrated separately in Figs. 5 and 6.

The lowest relevant value of c_1 is always $c_1 = 0$. Then the graph of $f(\bar{p}_1)$ touches the $\bar{p}_1$ axis from below at a skew root $R_1 = R_2 = 0$ and at an even double root $R_4 = R_6 = 3\alpha/4$; see Fig. 4. Increase of c_1 raises both these maxima above the axis, but the development is subtly different below and above the α bifurcation; see Figs. 5 and 6.

Below the α bifurcation, let us assume for definiteness that also $\alpha > 1/24\lambda'$ is given; see Fig. 4 for the significance of this. Then at small c_1 we have two small roots with $R_2 < R_1$; see Fig. 5(a). Upon raising c_1, they will have another confluence at $\bar{p}_1 = \Gamma$, and after that, they split in reverse order $R_1 < R_2$ as in Fig. 5(b). If we choose $\alpha < 1/24\lambda'$, the abscissa Γ lies to the left of the origin and the root ordering is as in Fig. 5(b) from the outset. When raising c_1 further, the simultaneous confluences $R_2 = R_4 = \alpha/4$ and $R_6 = R_3 = \alpha$ are formed at $c_1 = c^*_{1,\text{even}}$. Now a c_1 bifurcation takes place: at still higher c_1, R_2 and R_4 become complex whereas R_6 and R_3 emerge from α on the other side so that only R_1 and R_3 are left inside $[0,\alpha]$, see Fig. 5(c). The confluence $R_1 = R_3$ follows at $c_1 = c^{**}_{1,\text{odd}}$ which is the largest, physically possible value of c_1 when $\alpha < \alpha^*$.

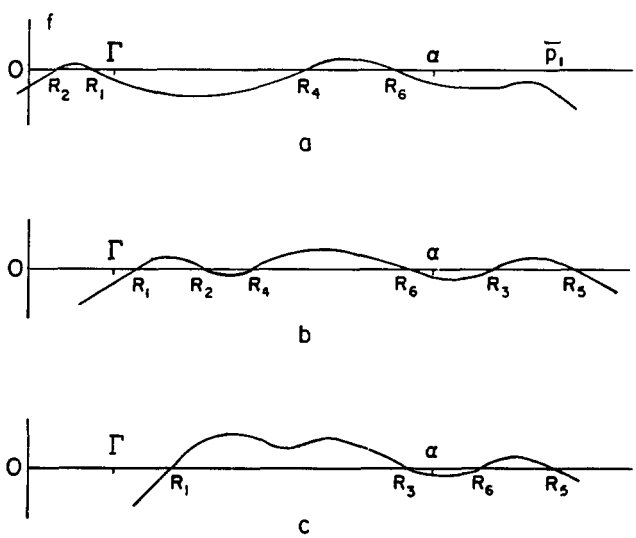

FIG. 5. Some significant stages in the development of the graph of $f(\bar{p}_1)$ below the α bifurcation, $\alpha < \alpha^* = 1/9\lambda'$ (schematic). The figures assume $\alpha > 1/24\lambda'$ so that Γ lies inside the interval $[0,\alpha]$. Three values of c_1 were chosen in the ranges: (a) $0 < c_1 < c^*_{1,\text{odd}}$; (b) $c^*_{1,\text{odd}} < c_1 < c^*_{1,\text{even}}$; (c) $c^*_{1,\text{even}} < c_1 < c^{**}_{1,\text{odd}}$.

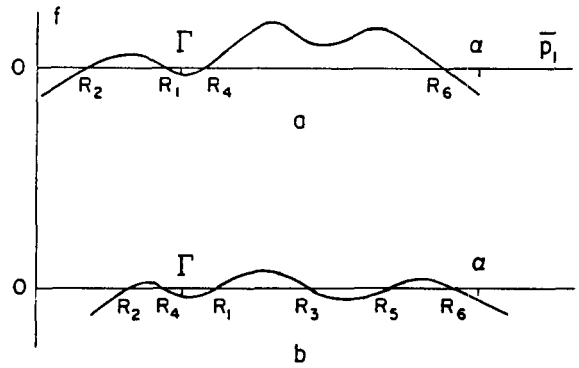

FIG. 6. Some significant stages in the development of the graph of $f(\bar{p}_1)$ above the α bifurcation, $\alpha^* = 1/9\lambda' < \alpha$ (schematic); Γ always lies within $[0,\alpha]$. Two values of c_1 were chosen in the following ranges: (a) $0 < c_1 < c^*_{1,\text{odd}}$; (b) $c^*_{1,\text{odd}} < c_1 < \min(c^*_{1,\text{even}}, c^{**}_{1,\text{odd}})$.

Above the α bifurcation, Γ always lies to the right of $\alpha/4$, while R_1 increases more rapidly than R_2, and a dip forms between R_4 and R_6 as in Fig. 6(a). At $c_1 = c^*_{1,\text{odd}}$ the confluence $R_1 = R_4 = \Gamma$ takes place, and simultaneously the dip touches the axis from above at $R_3 = R_5 = 7\alpha/10 + 1/30\lambda'$. At this first c_1 bifurcation, upon further increase of c_1, R_1 and R_4 emerge on the other side of Γ, and the odd second-order root splits as in Fig. 6(b). After that, three confluences are still possible. When $\alpha^* < \alpha < 1/4\lambda'$, it is seen from Eqs. (4.3) and (4.5) that $c^*_{1,\text{even}} < c^{**}_{1,\text{odd}}$ holds, and so we reach simultaneous confluences $R_2 = R_4 = \alpha/4$ and $R_5 = R_6 = \alpha$ at $c_1 = c^*_{1,\text{even}}$, followed by $R_1 = R_3 = \alpha/2$ at $c_1 = c^{**}_{1,\text{odd}}$, which is the largest possible value. When $\alpha > 1/4\lambda'$, the relation between $c^*_{1,\text{even}}$ and $c^{**}_{1,\text{odd}}$ is the opposite, and $R_1 = R_3$ occurs first at $c^{**}_{1,\text{odd}}$, followed by $R_2 = R_4$ and $R_5 = R_6$ at $c^*_{1,\text{even}}$, which now becomes the largest possible value of c_1. In either case, we have a second c_1 bifurcation between $c^*_{1,\text{odd}}$ and this largest value $c^{**}_{1,\text{odd}}$ or $c^*_{1,\text{even}}$.

VI. CATALOG OF MOTIONS

Amplitude-modulated motions of the odd–odd kind are easy to understand. As shown in Refs. 2 and 5, they are precessing ovals, possibly with change of shape as in Figs. 2(b) and 3(b), but without orbit reversal.

All other motions in this system are tied to one particular ridge or valley, and thus are threefold degenerate (with added mirror degeneracy about the ridge or valley). It turns out that under a 60° rotation the root parities of such a motion do not remain invariant. For instance, as will be shown presently, the libration in the 30° valley illustrated in Fig. 2(a) is even–even, but if we set up the same motion in the 90° valley over the η axis, it becomes even–odd. This degeneracy effect is a major nuisance in any algebraic discussion, and we shall try as much as possible to circumvent it by reference to graphs.

At the ends of their ranges, the amplitude-modulated motions degenerate into constant-amplitude motions at multiple roots of f. These c-a motions therefore play the role of demarcations between dynamical ranges; a graphical summary of all of them is given in Fig. 7.

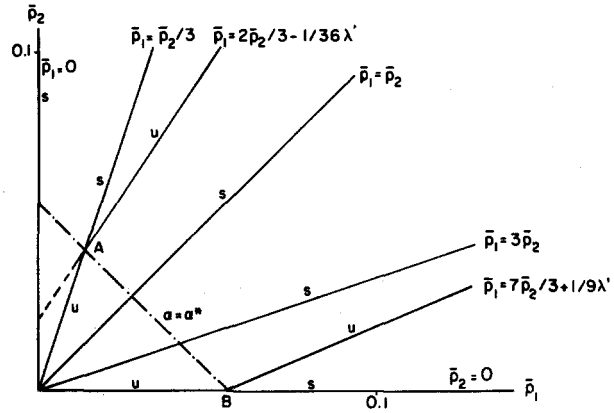

FIG. 7. A summary of all constant-amplitude motions in terms of their amplitudes $\bar{p}_1$ and $\bar{p}_2$ (to scale for $\lambda'=2$). Because of $\bar{p}_1+\bar{p}_2=\alpha$, motions with the same α lie on straight lines at 135° to the $\bar{p}_1$ axis; the line corresponding to the bifurcation $\alpha=\alpha^*$ is shown. Stable and unstable motions are labeled s and u, respectively. The three stable valley oscillations are represented by $\bar{p}_1=0$ (motion in the valley along the η axis) and $\bar{p}_1=3\bar{p}_2$ (corresponding to in-phase motion in the $+30°$ valley and to antiphase motion in the $-30°$ valley). The three top-of-the-ridge oscillations are $\bar{p}_2=0$ (motion along ridge over the ξ axis) and $\bar{p}_1=\bar{p}_2/3$ (corresponding to both the $+60°$ ridge and the $-60°$ ridge motions). These oscillations change stability at the bifurcation points B and A, respectively. The stable circular motion is represented by $\bar{p}_1=\bar{p}_2$. The three unstable elliptic motions that exist only above $\alpha=\alpha^*$ correspond to $\bar{p}_1=7\bar{p}_2/3+1/9\lambda'$ (stretched along the ξ ridge) and $\bar{p}_1=2\bar{p}_2/3+1/36\lambda'$ (representing both motions along the $+60°$ ridge and the $-60°$ ridge).

A. Motions with $c_1=0$

There are two algebraic possibilities arising from the two double roots at $\bar{p}_1=0$ and $3\alpha/4$, the former skew, the latter even.

The first one, $\bar{p}_1\equiv 0$, implies $\bar{p}_2\equiv\alpha$. The motion is harmonic and easily calculated from the equations of motion as

$$\xi\equiv 0,\quad \eta=(2\alpha)^{1/2}\cos\left[(1-\tfrac{3}{4}\alpha-\tfrac{15}{2}\lambda'\alpha^2)\rho+\text{const}\right], \tag{6.1}$$

where ρ denotes the (scaled) time as in Ref. 2. This is an obviously stable,[4] straight-line oscillation in the botton of the valley that lies along the η axis; technically, it is a Case (I) c-a motion of familiar type.[3–5]

The second one, $\bar{p}_1\equiv 3\alpha/4$, implies $\bar{p}_2\equiv\alpha/4$. Since the root is even, this is a Case (II)[3–5] with a fixed phase relation $\cos(2\bar{q}_1-2\bar{q}_2)\equiv+1$, or $\bar{q}_1-\bar{q}_2\equiv 0,\pi$. There are now two harmonic straight-line motions with the same frequency as in (6.1), but with a $1:\sqrt{3}$ amplitude ratio and their components in phase or in antiphase, i.e., they are oscillations in the bottom of the $+30°$ and the $-30°$ valley, respectively. In Fig. 7 these stable valley oscillations are represented by the lines $\bar{p}_1=0$ and $\bar{p}_1=3\bar{p}_2$.

Increasing the amplitude of any of these oscillations will eventually lead to an obvious soliton solution connecting two opposite saddles of the potential via a straight path.

B. Motions below c_1 bifurcation

Slight increase of c_1 beyond zero changes the straight-line valley bottom oscillations into narrow oval librations about the bottoms. The one about the η axis is even–odd because in this orbit orientation a steady increase of the relative phase is required.[2,5] The two in the $\pm 30°$ valleys are even–even, with the phase difference oscillating around 0 and π, respectively.[2,5] Thus algebraically the three equivalent motions appear quite different; however, the complication also harbors some insights.

First take the $\pm 30°$ librations. They evolve from the straight-line motion at the root $\bar{p}_1=3\alpha/4$ which for $0<c_1<c_{1,\text{odd}}^*$ splits into the pair $R_{4,6}$ of Figs. 5(a) and 6(a). Their evolution as c_1 grows appears uneventful; two particular cases are shown in Figs. 2(a) and 3(a). Still, there are some minor features which we do not think important enough to derive in print, but which can be glimpsed from the dynamically identical η-axis libration.

The libration in the η valley evolves from the straight-line motion (6.1) at the skew double root $\bar{p}_1\equiv 0$ which for $0<c_1<c_{1,\text{odd}}^*$ splits into two roots R_1 and R_2. It then makes a difference whether the given α lies above or below $1/24\lambda'$, as emphasized in Secs. IV and V and in Fig. 4. If $\alpha<1/24\lambda'$, then the critical value $\alpha=2\alpha/5-1/60\lambda'$ lies outside the interval $[0,\alpha]$, and $R_1<R_2$ always holds. Nothing remarkable happens as c_1 grows towards its bifurcation value. If $\alpha>1/24\lambda'$, however, Γ lies inside $[0,\alpha]$ as shown in Fig. 5. As c_1 is now increased from zero onwards, we have first $R_2<R_1$ and later $R_1<R_2$ as above. It can be shown that there is a corresponding minor change in orbit shape. At the intermediate state $R_1=R_2=\Gamma$ it can furthermore be shown that the envelope of the libration is a rectangle with straight sides. This motion appears paradoxical, for at the *double* root Γ the amplitudes must be constant. Indeed they are, but as we have elaborated elsewhere, for this c-a motion at a *skew* double root *inside* the interval $[0,\alpha]$ the phase difference between the two degrees of freedom is not constant so that no stable closed orbit results and a libration persists; see Ref. 5, Sec. IV D, Theorem 6 *et seq.* Exactly the same change of orbit shape and the same intermediate stage in a rectangle take place in the $\pm 30°$ librations, of course, but are not announced by algebraic peculiarities.

These valley librations have characteristic turning points where the motion comes to instantaneous rest.[2,5] In Figs. 2(a) and 3(a), such turning points are used as natural beginnings of the graphs. The motion begins as a narrow oval which slides down towards the valley and widens as it does so, narrows again as it climbs the other slope of the valley, then comes to a stop, reverses, and so on. When c_1 increases towards its bifurcation value, the development of the librating orbit is noticeably different below and above the α bifurcation, as is readily understood from Figs. 4–6, and considering for simplicity only the 30°-libration amplitude-modulated between R_4 and R_6.

Below the α bifurcation, see Fig. 4 and Fig. 5(b), the amplitude at both ends of its modulation range tends towards double roots $R_6=R_3=\alpha$ and $R_4=R_2=\alpha/4$. Thus the motion tends from a long-lasting stage in an almost straight line close to the ξ-axis ridge to an analogous stage

close to the 60° ridge, with a briefer oval stage in between, and back. At the bifurcation value $c_1 = c^*_{1,\text{even}}$ the motion converts in infinite time between straight-line stages over the ridges.

Above the α bifurcation, a double root approaches in the middle of the modulation range, $R_3 = R_5 = 7\alpha/10 + 1/30\lambda'$, see Fig. 4 and Fig. 6(a). Now the fairly straight stages close to the ridges last briefly, whereas the oval intermediate stage in the valley lasts long and becomes rather more circular. At the bifurcation value $c_1 = c^*_{1,\text{odd}}$ the motion converts in infinite time from an oval stage in the valley through a brief stage close to a ridge, back to a valley oval described in the opposite sense.

In Figs. 2(a) and 3(a) this different evolution of the two valley librations can be anticipated clearly in the different envelopes of the orbit, with a slim and a bulging waist, respectively.

C. Motions above c_1 bifurcation

When c_1 is raised a little over the bifurcation value, the energy becomes large enough for the motion to cross over the potential ridges. The two valley librations just described then become the narrow and the wide precessions illustrated in Figs. 2(b) and 3(b), respectively. Both are odd–odd, without turning points, and can only be set up from an initial condition with nonvanishing velocity.[2,5]

Above the α bifurcation, see Fig. 6(b), there are still two more amplitude modulations possible: one even–even, having $\bar{p}_1$ within the range $[0,\Gamma]$, the other even–odd, with $\bar{p}_1$ not far from α all the time. These correspond to three librations, similar to the ones with the even–odd and even–even ranges in Fig. 5(a), but this time the orbit librates over a ridge, not in a valley. Figure 3(c) illustrates a typical instance.

Raising c_1 still further, again above the α bifurcation, we encounter the second c_1 bifurcation described at the end of Sec. V. In case $\alpha^* < \alpha < 1/4\lambda'$, at $c_1 = c^*_{1,\text{even}}$ the double roots $R_2 = R_4 = \alpha/4$ and $R_5 = R_6 = \alpha$ are reached. The ridge librations then contract into straight-line motions right on top of the ridges; astonishingly enough, they are dynamically stable, as is seen at once from Fig. 6(c). Increasing the amplitude of these motions again leads eventually to an obvious straight-line solution connecting two opposite hilltops. In the second case, $\alpha > 1/4\lambda'$, the confluence $R_1 = R_3 = \alpha/2$ takes place at $c_1 = c^{**}_{1,\text{odd}}$. Now the precession becomes circular.

D. Motions at maximum c_1

For all $\alpha < 1/4\lambda'$, c_1 reaches its physically possible maximum at $c^{**}_{1,\text{odd}}$ when $R_1 = R_3 = \alpha/2$ and no other real roots of $f(\bar{p}_1)$ are left on $[0,\alpha]$. The corresponding motion is circular, uniform, and stable; in Fig. 7 it is represented by the line $\bar{p}_1 = \bar{p}_2$.

For $\alpha > 1/4\lambda'$ this motion is still possible, but the maximum of c_1 is now $c^*_{1,\text{even}}$, see Fig. 4, and the c-a motions at the corresponding even–even and even–odd double roots are stable, harmonic hence-and-forth oscillations on top of the ridge backs; in Fig. 7 they are represented by the lines $\bar{p}_1 = \bar{p}_2/3$ and $\bar{p}_2 = 0$ (or $\bar{p}_1 = \alpha$).

E. Summaries

Figure 8 summarizes the various bifurcations graphically in a plot of c_1/α^2 vs $\lambda'\alpha$, based on Eqs. (4.3)–(4.6).

As a complement to the bifurcations, we may also ask for representative initial conditions which will produce the various motions. The subject is treated briefly in Ref. 2, and with great generality in Ref. 5. It is particularly easy to set up a motion at a time when its amplitude modulation is at an even root, for it then goes to rest in the (ξ,η) plane. The release points for the various librations are easily calculated, following Ref. 2, and are reproduced in Fig. 9.

The precessions, which never come to rest, can be set up, for instance, by release from a point on the positive ξ axis with a purely transverse velocity $\dot{\eta}$. The amplitude is then at an odd root. Figure 10 shows the pertinent value of $\dot{\eta}$ plotted against ξ. As an incidental result, the same plot also yields other motions having an odd root of the amplitude modulation which corresponds to a transverse crossing of the ξ axis: the ridge libration over the ξ axis, and the valley libration along the η axis.

F. Complements on the c_1 bifurcation

When $\alpha < \alpha^*$ the c_1 bifurcation occurs at $c^*_{1,\text{even}}$ with a graph of $f(\bar{p}_1)$ intermediate between Figs. 5(b) and 5(c), having two double roots $R_2 = R_4$ and $R_3 = R_6$ where the

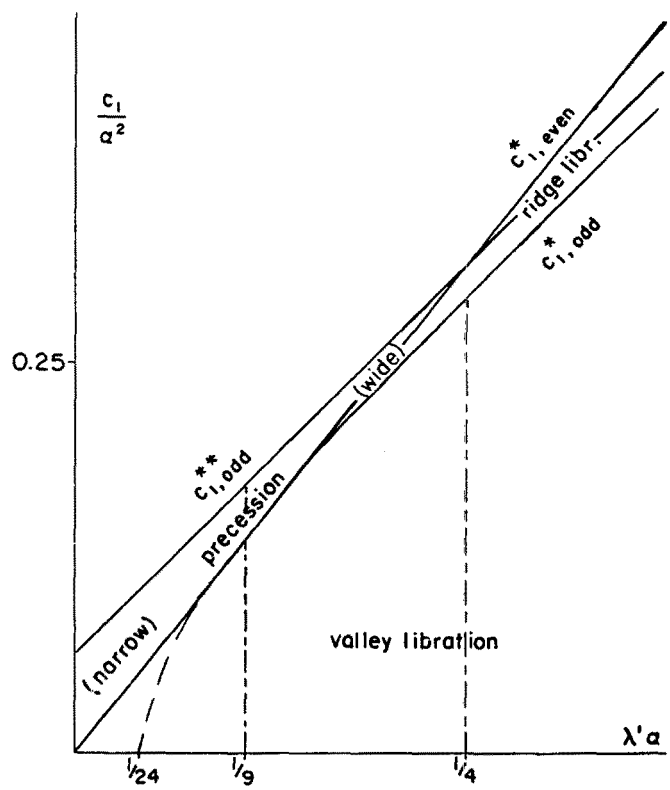

FIG. 8. Graphical summary of bifurcation values of c_1 and α. In these plots of c_1/α^2 vs $\lambda'\alpha$, $c^*_{1,\text{even}}$ and $c^{**}_{1,\text{odd}}$ are represented by straight lines given by Eqs. (4.3) and (4.5). The $c^*_{1,\text{odd}}$ appears almost straight, but it is curved, see Eq. (4.4), and makes a contact at the α bifurcation value α^*; it continues towards the left as the dashed line which demarcates a minor shape difference between the valley librations, as mentioned in Sec. VI B.

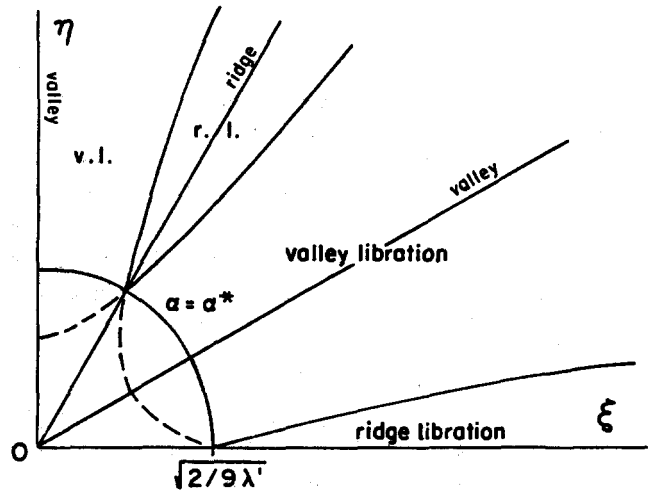

FIG. 9. Representative initial conditions at an even root: release from rest in the (ξ,η) plane, to yield librations in valleys and over ridges. To obtain the complete figure with sixfold symmetry, adjoin mirror images on the left, and below the ξ axis. Constant values of α lie on circles about the origin; the bifurcation circle for α^* is shown. The broken lines demarcate the minor shape difference of the valley librations mentioned in Sec. VI B.

curve touches the $\bar{p}_1$ axis from *above*. The corresponding c-a motions are evidently oscillations on top of the ridges which coexist with the conversion motions leading towards a ridge, and they are orbitally unstable because the slightest change in c_1 results in either a valley libration or a precession. They correspond to the "unstable" parts of the lines $\bar{p}_1 = \bar{p}_2/3$ and $\bar{p}_2 = 0$ in Fig. 7. Entirely analogous, unstable ridge oscillations occur in the $N = 4$ system for the parameter range $1 < \lambda < 3$ (Ref. 2).

When $\alpha > \alpha^*$ the c_1 bifurcation occurs at $c^*_{1,\text{odd}}$ and exhibits unexpected features which can only be understood

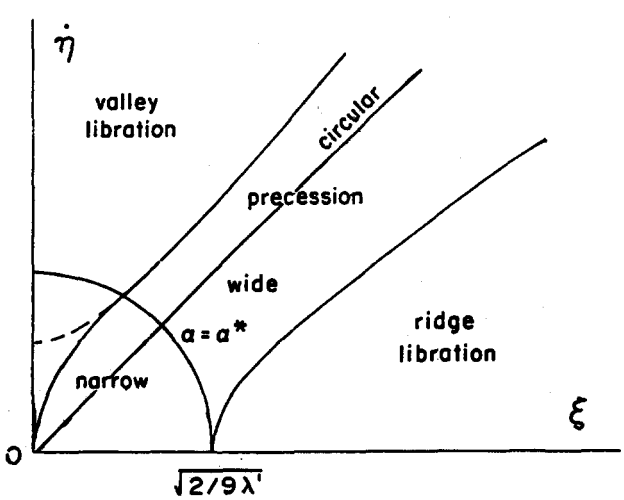

FIG. 10. Representative initial conditions at an odd root: transverse launch upwards from the ξ axis, to yield counterclockwise precessions, librations over the ξ ridge, and librations in the η valley. Constant values of α lie on circles about the origin; the bifurcation circle for α^* is shown. The broken line demarcates the minor shape difference of the valley librations mentioned in Sec. VI B.

with reference to the general theory of relative phases developed in Ref. 5, especially Sec. IV D 4. The graph intermediate between Figs. 6(a) and 6(b) has the odd double root $R_3 = R_5$ and the skew $R_1 = R_4 = \Gamma$. The c-a motion at the former is readily seen to be an ellipse stretched along the ξ ridge. The c-a motions at Γ must likewise be elliptical but over the $\pm 60°$ ridges, on account of the symmetry degeneracy. However, the motions neighboring to these ridge ellipses at values of c_1 slightly below $c^*_{1,\text{odd}}$ are all valley librations with long-lasting elliptical stages in the *valleys*, not along the ridges. The explanation of the paradox is that the relative phase of an *unstable* c-a motion at a *skew* root *inside* $[0,\alpha]$ is *not* continuous with the relative phase of the neighboring motions, see *l.c.* Theorem 4. As $c_1 \to c^*_{1,\text{odd}}$ from below, the orbit accordingly shifts in a discontinuous manner from an orientation mainly along a valley, to a permanent orientation along a ridge. It does so for the odd–odd motion over the ξ ridge as well, of course, but in this case the discontinuity arises from the sudden contact of the dip in Fig. 6(a) with the axis, and cannot be deduced from the quoted, general theorem which applies at the skew root Γ only.

These remarkable elliptic motions are represented by the lines $\bar{p}_1 = 2\bar{p}_2/3 - 1/36\lambda'$ and $\bar{p}_1 = 7\bar{p}_2/3 + 1/9\lambda'$ in Fig. 7. They are orbitally unstable, and coexist with obvious conversion motions that tend to any of the elliptic orbits. As c_1 is raised above $c^*_{1,\text{odd}}$, *two* different developments are possible, depending on the phase changes which are imposed at the same time. In one, the ellipse stretches out along the ridge, and a ridge libration results. This sequence is reminiscent of the c_1 bifurcation in the $N = 4$ system with $\lambda > 3$ (where the ellipse reduces to a circle).[2] However, the ellipse can also shrink in the ridge direction, and then a (wide) precession results.

The complicated course of the c_1 bifurcation above $\alpha = \alpha^*$ is not merely an artifact of the slow-fluctuation method; we have verified it by means of numerical integrations of the exact equations of motion in the potential (2.1).

G. Complements on the α bifurcation

When $\alpha = \alpha^*$ and also $c_1 = c^*_{1,\text{even}} = c^*_{1,\text{odd}}$, then $f(\bar{p}_1)$ possesses two skew third-order roots: $R_1 = R_2 = R_4 = \alpha/4 = \Gamma$ and $R_3 = R_5 = R_6 = \alpha$, see Fig. 4 and also Fig. 7 where these confluences correspond to the points A and B. The corresponding c-a motions are top-of-the-ridge oscilla-

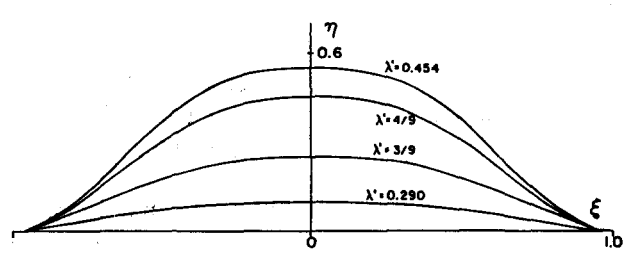

FIG. 11. The orbit of the curved soliton connecting the opposite hilltops at $(-1,0)$ and $(+1,0)$ for selected values of λ'. The initial values of $\eta(0)$ are 0.098 8445, 0.254 5752, 0.456 4851, 0.552 3317.

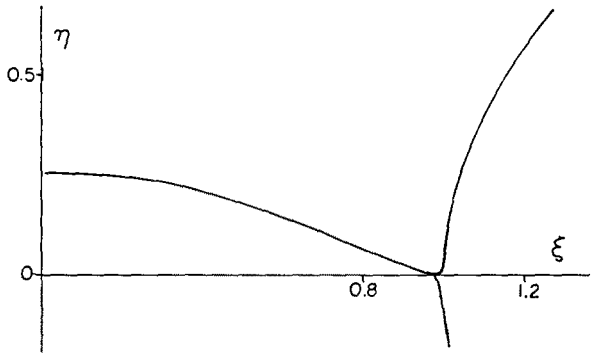

FIG. 12. Two orbits bracketing the curved soliton for $\lambda' = \frac{1}{3}$. The initial values of $\eta(0)$ are 0.254 0000 and 0.255 0000.

tions, and are clearly unstable. There are also conversion motions tending towards these. Qualitatively, all these motions are similar to the ones at c_1 bifurcation below α^*. However, above α^* the ridge oscillation is found to be orbitally stable, whereas the aforementioned, elliptic ridge orbit has emerged out of the ridge oscillation below α^*, and has inherited the latter's instability. This is a typical α bifurcation pattern; see Ref. 6 for a general description.

VII. SOLITONS

The obvious, straight-line soliton solutions connecting two opposite saddles or two opposite hilltops are beyond the range of validity of the slow-fluctuation method, but as mentioned earlier, they are reached by a natural extrapolation of oscillatory straight-line solutions at much smaller amplitudes. It is one of the fringe benefits of the method that other c-a solutions, too, can by extrapolation yield clues to the existence of solitons which may be of quite unexpected nature.

Begin with the elliptic top-of-the-ridge motions described in Sec. VI F. For the sake of discussion, take the one over the ξ axis. When its amplitude is increased, it need not remain elliptical, but the orbit should remain a closed curve with mirror symmetry about the η axis. In the limit, its extremes should reach the two hilltops at $(-1,0)$ and $(+1,0)$. Thus, the existence of a curved soliton connecting opposite hilltops is worth investigating. This was done numerically. The condition "rest at hilltop" determines the total energy; an orbit can then be launched transversely from the η axis with the velocity corresponding to the given energy and the initial $\eta(0)$, and can be calculated from the exact equations of motion. By trial, error, and interpolation between over- and undershoot, we did indeed find curved soliton solutions which bear a slight similarity to one known[9] in the $N = 2$ system. Some orbits are reproduced in Fig. 11. This curved soliton exists only for a finite range of values of λ', from 0.283 to 0.454 (to three decimals). The lower bound is expected because of the lower bound $\lambda' = 1/9\alpha$ for the elliptic slow-fluctuation solutions (which would become $\lambda' = 2/9$ if the slow-fluctuation method were still valid for a motion coming to rest at a hilltop). The upper bound results because at high λ' the required $\eta(0)$ can no

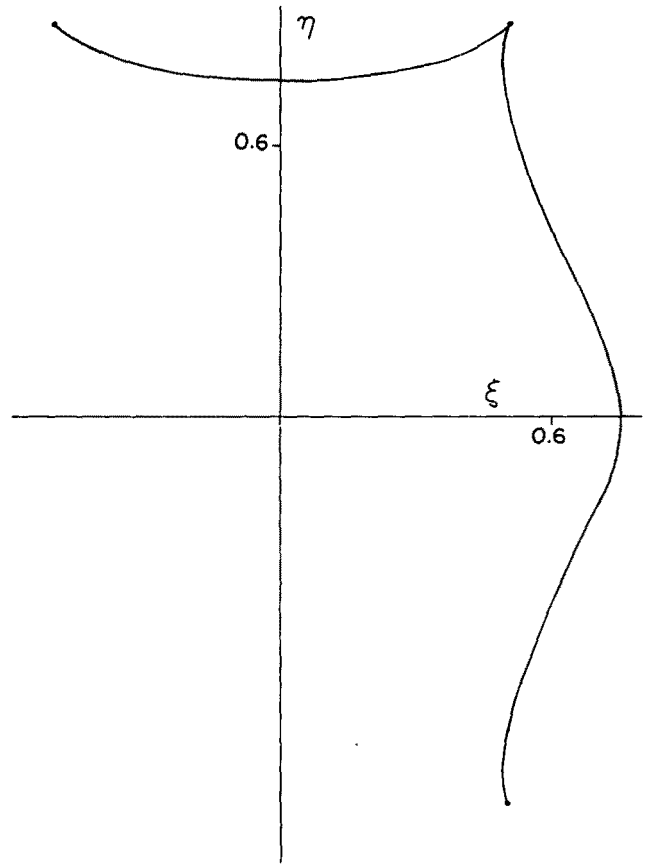

FIG. 13. Two curved solitons connecting nonopposite hilltops when $\lambda' = \frac{1}{3}$. The one symmetrical about the η axis was initiated from $\eta(0) = 0.745\,253\,55$; the one symmetrical about the ξ axis was launched from $\xi(0) = 0.755\,683\,38$.

longer lie between the two saddles on the η axis. This range of allowed values is rather narrow; the curved soliton might easily be overlooked without the hint from the slow-fluctuation method. We emphasize that this kind of numerical experimentation requires fairly high precision because of the solitons' evident instability. In Fig. 12 we show for $\lambda' = 3/9$ two orbits launched with a difference of only 0.001 in $\eta(0)$ which remain virtually indistinguishable from the true soliton up to almost the hilltop, but then veer off sharply in opposite directions.

In a similar fashion we may extrapolate from the circular precessions of the slow-fluctuation catalog. Such an orbit could at larger amplitudes become somewhat hexagonal, possibly also triangular. Accordingly, one may surmise the existence of curved solitons connecting a hilltop with an adjacent and with a next-but-one hilltop. Such solitons exist, in fact, and examples for $\lambda' = 3/9$ are shown in Fig. 13. We confine ourselves to this demonstration and leave out all further detail.

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On head-wave amplitudes

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The head-wave contribution to a reflection is investigated by two different methods and it is shown that the new result presented by Lerche and Hill [J. Math. Phys. **26**, 1420 (1985)] for the head-wave amplitude is in error due to the use of an inappropriate mathematical method.

I. INTRODUCTION

In a recent paper, Lerche and Hill[1] have investigated the amplitudes of reflections and head waves from a rough interface. As a prerequisite, they considered a smooth interface and derived an asymptotic result for the amplitude of the head-wave contribution (LH30—henceforth we use the abbreviation LH to refer to Lerche and Hill and equations therein). They comment that their result differs from the expression in Aki and Richards[2] [Eq. (6.25)] by a factor $(2/e)^{1/2}$ and that the evaluation of Aki "involves further approximations whereby the factor $(2/e)^{1/2}$ is lost." This result and statement are surprising as the asymptotic results for the head-wave amplitude derived by a variety of distinct techniques, e.g., asymptotic ray theory,[3] Cagniard–de Hoop–Pekeris method[4–8] as well as the usual branch cut evaluations by asymptotic techniques,[2,9,10] agree. Incidentally, we find that expression (LH30) is in error by a factor of $(2e)^{-1/2}$ [not $(2/e)^{1/2}$], as the result in Aki and Richards[2] also contains an error of a factor of 2. In this paper, we rederive the head-wave amplitude by two techniques (to establish beyond doubt the correct result) and identify the source of error in LH.

II. BRANCH-CUT EVALUATION

The expression for the pressure field of the reflected wave is given by

$$P_{\text{refl}} = i\int_0^\infty B\,\frac{J_0(KR)e^{ik_1(z+z_0)}}{k_1}K\,dK, \qquad \text{(LH6)}$$

where the variables are defined in LH and for brevity we have not substituted for the reflection coefficient, B (LH5). This integral can be decomposed and the head-wave contribution comes from the term

$$I_2 \simeq e^{-i(\pi/4)}\left(\frac{\omega s_1}{2\pi R}\right)^{1/2}\int_0^{\pi_2}\frac{d\theta\cos\theta(\sin\theta)^{1/2}}{a+b\sin^2\theta}\times(\sin^2\theta_c-\sin^2\theta)^{1/2}e^{iN\cos(\theta-\phi)} \qquad \text{(LH14)}$$

$$= e^{-i(\pi/4)}\left(\frac{\omega s_1}{2\pi R}\right)^{1/2}\int_0^{\pi_2}\frac{d\theta\cos\theta(\sin\theta)^{1/2}}{a+b\sin^2\theta}\times\exp[iN\cos(\theta-\phi)+\tfrac{1}{2}\ln(\sin^2\theta_c-\sin^2\theta)], \qquad \text{(LH18)}$$

where, using LH's notation, we have made some trivial substitutions to simplify. LH evaluated the second expression (LH18) by finding the stationary points of the exponent. The traditional method of evaluating the branch cut integral in expression (LH14) is to change the variable of integration to the branch cut radical,[9,10] i.e.,

$$\nu = (\sin^2\theta_c - \sin^2\theta)^{1/2} \qquad (1)$$

and convert it to a saddle-point integral. With this substitution (1), the exponent in (LH14) becomes

$$\chi = iN[\cos\phi(1-\sin^2\theta_c+\nu^2)^{1/2} + \sin\phi(\sin^2\theta_c-\nu^2)^{1/2}], \qquad (2)$$

which has a stationary point, i.e., $d\chi/d\nu = 0$ at $\nu = 0$. At this saddle point we have

$$\chi = iN\cos(\phi-\theta_c)$$

and

$$\frac{d^2\chi}{d\nu^2} = -\frac{iN\sin(\phi-\theta_c)}{\sin\theta_c\cos\theta_c}. \qquad (3)$$

The integral can be evaluated using the principle of stationary phase without distorting the path of integration which runs from $\nu = \sin\theta_c$ to $\nu = 0$ and then to $\nu = i\cos\theta_c$. Using the second-order saddle-point method, we obtain the asymptotic result

$$I_2 \simeq -\frac{1}{\omega s_1}\cdot\frac{\sin\theta_c}{R^{1/2}}\left(\frac{\cos\theta_c}{\mu\sin(\phi-\theta_c)}\right)^{3/2}\times\frac{\exp[iN\cos(\theta_c-\phi)]}{a+b\sin^2\theta_c}. \qquad (4)$$

This expression should be compared with (LH27) and is seen to differ by a factor $-(2e)^{1/2}$ [the negative sign appears to be a trivial error corrected in (LH30)]. The expression for the head-wave contribution is then

$$P_{\text{head}} = \frac{i}{\omega}\cdot\frac{2\rho_1}{\rho_2}\cdot\frac{s_2}{s_1^2-s_2^2}\cdot\frac{\exp(i\omega\tau_h)}{R^{1/2}L^{3/2}} \qquad (5)$$

compared with (LH30). This expression (5) agrees with Aki and Richards[2] [Eq. (6.25)] apart from a factor of 2 that has been lost between Eqs. (6.23) and (6.24) of that book. Next we discuss why LH's evaluation is in error and then confirm expression (5) by another method.

III. SADDLE-POINT EVALUATION

To evaluate expression (LH18), LH first determine the stationary points of the exponent. The significant one exists at

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$$\theta_2 = \theta_c + i/2N \sin(\phi - \theta_c) + O(N^{-2}) \qquad \text{(LH22)}$$

and the second derivative is

$$\frac{d^2\psi}{d\theta^2} = 2N^2 \sin^2(\theta_c - \phi) + O(N). \qquad \text{(LH26)}$$

The contour of integration is distorted to pass through the saddle point θ_2 and the integral evaluated by the saddle-point method. Unfortunately, although θ_2 is a stationary-phase point, the saddle-point method is inappropriate. A basic requirement for the saddle-point method is that the Taylor expansion of the exponent at the stationary-phase point should be a good approximation within the width of the saddle point where the main contribution to the integral arises. From the second derivative of the exponent (LH26), we see that the width of saddle is of order $1/|N \sin(\theta_c - \phi)|$. Higher derivatives of the exponent are given by

$$\frac{d^n\psi}{d\theta^n} = -\frac{1}{2}(n-1)!(2iN)^n \sin^n(\phi - \theta_c)[1 + O(N^{-1})]. \qquad (6)$$

It is readily apparent that within the width of the saddle point, all terms in a Taylor expansion of the exponent are of similar magnitude and importance. Notice that the distance between the saddle point θ_2 (LH22) and the branch point θ_c is comparable with the saddle width, and at the branch point the exponent is singular. The Taylor expansion is therefore not valid over the required range. The saddle-point method cannot be used to evaluate the integral and LH's result (LH27) is in error. Rather than leading to a "small" correction by $(2/e)^{1/2}$, their technique is inappropriate and leads to a significant error of $(2e)^{-1/2}$.

LH have evaluated the integral I_2 by a technique equivalent to the Stirling approximation for the gamma function. Then we have

$$\Gamma(n+1) = \int_0^\infty x^n e^{-x}\, dx \qquad (7a)$$

$$\simeq n^n e^{-n} \int_{-\infty}^{\infty} e^{-(1/2n)(x-n)^2}\, dx \qquad (7b)$$

$$= (2n\pi)^{1/2} n^n e^{-n}. \qquad (7c)$$

Expression (7a) is the integral definition of the gamma function which is evaluated by the second-order saddle point approximation (7b) to give the Stirling approximation (7c). This approximation is valid for $n \gg 1$ when the saddle point at $x = n$ is well away from the origin. But for $n = \frac{1}{2}$, we know $\Gamma(\frac{3}{2}) = \pi^{1/2}/2$ exactly, whereas the Stirling approximation (7c) gives $(\pi/2e)^{1/2}$, i.e., a factor of $(2/e)^{1/2}$. The other factor of 2 comes from approximating the integral on both sides of the branch point by the semi-infinite integral [as in (7a)].

IV. THE CAGNIARD–DE HOOP–PEKERIS METHOD

An alternative technique for investigating the head-wave contribution is the Cagniard–de Hoop–Pekeris method.[4–8] Rather than evaluate (LH6) asymptotically, we take the inverse Fourier transform with respect to frequency and obtain the impulse response. The head-wave contribution can then be investigated by a first-motion approximation, i.e., a Taylor expansion about the head-wave discontinuity, and is found to be the inverse Fourier transform of (5).

We outline very briefly the Cagniard technique. Using the symmetries of the Bessel function, expression (LH6) can be rewritten (ω real)

$$P_{\text{refl}} = \frac{i|\omega|}{2} \int_{-\infty}^{\infty} B \frac{H_0^{(1)}(\omega p R) e^{i\omega q_1 (z+z_0)}}{q_1} p\, dp, \qquad (8)$$

where $\omega q_1 = k_1$ and $\omega p = K$. The p-contour is distorted so that $\text{Im}(pR + q_1(z+z_0)) = 0$, the so-called Cagniard contour. We use

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} H_0^{(1)}(a\omega) e^{-i\omega t}\, d\omega = \begin{cases} -\dfrac{2i}{\pi(t^2 - a^2)^{1/2}}, & \text{for } |t| > a, \\ 0, & \text{for } |t| < a, \end{cases} \qquad (9)$$

to take the inverse Fourier transform of (8) and obtain

$$P_{\text{refl}} = \frac{2}{\pi} \cdot \frac{d}{dt} \text{Im} \int_{c_-} \frac{Bp}{q_1} \frac{H(t - pR - q_1(z+z_0))}{[(t - q_1(z+z_0))^2 - p^2R^2]^{1/2}}\, dp, \qquad (10)$$

where by symmetry we have restricted the Cagniard contour to the fourth quadrant. This expression is zero for $t < \tau_h$ (as all terms in the integrand are real) and nonzero for $t > \tau_h$ as B becomes complex at the branch point, $p = s_2$. Expanding about $p = s_2$ for $t \gtrsim \tau_h$, the important terms in the integrand are for the factor $(p - s_2)^{1/2}$ from the branch cut in B, and $(t - \tau_h - L(p - s_2))^{-1/2}$ from the denominator. Treating the other terms as constant and evaluating the integral, we obtain

$$P_{\text{head}} \simeq -\frac{2\rho_1}{\rho_2} \cdot \frac{s_2}{s_1^2 - s_2^2} \cdot \frac{1}{R^{1/2} L^{3/2}} H(t - \tau_h), \qquad (11)$$

which is consistent with the inverse Fourier transform of (5). Including higher-order terms in the Taylor expansion of the integrand (10) results in contributions to the head wave with higher-order discontinuities, e.g., $(t - \tau_h) \times H(t - \tau_h)$, but this does not modify the asymptotic result (5).

V. CONCLUSIONS

It has been shown that the new result given by Lerche and Hill[1] for the head-wave contribution to a reflection is incorrect by a factor $(2e)^{-1/2}$. The correct result is confirmed using two different but standard techniques. The error occurred in Lerche and Hill due to the inappropriate use of the saddle-point method. Their method is equivalent to using the Stirling approximation for $\Gamma(n+1)$ with $n = \frac{1}{2}$ [introducing an error of $(2/e)^{1/2}$] and reducing an integral on both sides of the branch point to one side (causing a further error of $\frac{1}{2}$). Fortunately the error in Sec. II of LH does not affect the rest of the paper. The results in Sec. III are still valid.[11]

ACKNOWLEDGMENTS

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A search for bilinear equations passing Hirota's three-soliton condition. I. KdV-type bilinear equations

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In this paper the results of a search for bilinear equations of the type $P(D_x, D_t)F \cdot F = 0$, which have three-soliton solutions, are presented. Polynomials up to order 8 have been studied. In addition to the previously known cases of KP, BKP, and DKP equations and their reductions, a new polynomial $P = D_xD_t(D_x^2 + \sqrt{3}D_xD_t + D_t^2) + aD_x^2 + bD_xD_t + cD_t^2$ has been found. Its complete integrability is not known, but it has three-soliton solutions. Infinite sequences of models with linear dispersion manifolds have also been found, e.g., $P = D_x^M D_t^N D_y^P$, if some powers are odd, and $P = D_x^M D_t^N (D_x^2 - 1)^P$, if M and N are odd.

I. INTRODUCTION

There are several methods for studying integrable nonlinear evolution equations (NEE's), the most famous being the inverse scattering method. However, there are still no systematic methods to approach NEE's that are not completely integrable, but which nevertheless do have some nice properties. Such "almost integrable" systems may be quite important in practice. For these the heavy machinery associated with complete integrability may not be applicable. It is therefore useful to study also other approaches where less demanding assumptions can be made.

One interesting alternative method was introduced by Hirota[1] 15 years ago (for reviews see, e.g., Refs. 2 and 3). The fundamental idea in Hirota's formalism is to use some *dependent variable transformation* to put the equation in a form where the unknown function appears *bilinearly*. In the process one usually has to extract one or two derivatives. For example in the case of the Korteweg–de Vries equation

$$u_{xxx} - 6uu_x + u_t = 0, \tag{1}$$

one first introduces a new dependent variable v by $u = v_x$. Then (1) can be written as

$$\partial_x [v_{xxx} - 3(v_x)^2 + v_t] = 0. \tag{2}$$

Finally with the dependent variable transformation[1]

$$u = -2\,\partial_x^2 \log F \tag{3}$$

or $v = -2\,\partial_x \log F$, we find that the part in square brackets in (2) vanishes provided that F satisfies the equation

$$(D_x^4 + D_xD_t)F \cdot F = 0, \tag{4}$$

where the operators D_x and D_t are defined by

$$P(D_x, D_t)F \cdot F = P(\partial_x - \partial_{x'}, \partial_t - \partial_{t'})F(x,t)F(x',t')|_{x'=x,\,t'=t}, \tag{5}$$

for an arbitrary polynomial P. (For a list of properties of the D operator, see Appendix I of Ref. 4.)

A bilinear form has been constructed for many other completely integrable systems by Hirota and others. From their results one can make the conjecture that all completely integrable NEE's can be put into a bilinear form (this will sometimes involve auxiliary independent and dependent variables, see below). The converse, however, is not true: a bilinear form can also be constructed for many equations that are not integrable. To be precise, the bilinear formulation guarantees only the existence of two-soliton solutions (see Sec. II). So in this sense Hirota's bilinear formalism is somewhere between complete integrability and complete arbitrariness.

In this paper we report the results of a search for bilinear equations of type

$$P(D_x, D_t)F \cdot F = 0, \tag{6}$$

which have three-soliton solutions. To set the stage we list here those previously known completely integrable NEE's that lead to bilinear equations of type (6). For the Boussinesq equation

$$u_{xxxx} + 6(u^2)_{xx} + u_{xx} - u_{tt} = 0, \tag{7}$$

one uses the dependent variable transformation

$$u = \partial_x^2 \log F, \tag{8}$$

and after extracting two x derivatives [cf. (2)] one obtains[5,6]

$$(D_x^4 + D_x^2 - D_t^2)F \cdot F = 0. \tag{9}$$

For the Sawada–Kotera equation[7]

$$u_{xxxxx} - 15uu_{xxx} - 15u_xu_{xx} + 45u^2u_x + u_t = 0, \tag{10}$$

the substitution (3) and extraction of one x derivative yields[7,8]

$$(D_x^6 + D_xD_t)F \cdot F = 0. \tag{11}$$

The shallow water wave equation of Hirota and Satsuma[9]

$$u_{xxt} + 3uu_t - 3u_x \int_x u_t\,dx' - u_x - u_t = 0, \tag{12}$$

yields with (8)

$$(D_x^3D_t - D_x^2 - D_xD_t)F \cdot F = 0. \tag{13}$$

The above equations have two independent variables, x and t, but bilinear equations have also been constructed for some $(2+1)$-dimensional equations. The most famous of these is the Kadomtsev–Petviashvili (KP) equation

$$u_{xxxx} + 6(u^2)_{xx} + u_{xt} \pm 12u_{yy} = 0, \tag{14}$$

which yields with (8) (Ref. 10)

$$(D_x^4 + D_xD_t \pm 12D_y^2)F \cdot F = 0. \tag{15}$$

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The bilinear form of a given integrable NEE is not always as simple as the ones given above. For the modified KdV equation

$$v_t + 6v^2 v_x + v_{xxx} = 0\,, \tag{16}$$

Hirota proposes[3,11] the independent variable transformation

$$v = -i\,\partial_x \log\,(f/f^*)\,, \tag{17}$$

which yields a *pair* of bilinear equations

$$(D_t + D_x{}^3) f\cdot f^* = 0\,,$$
$$D_x{}^2 f\cdot f^* = 0\,, \tag{18}$$

for the two dependent functions, f and its complex conjugate.

Completely integrable NEE's come in hierarchies and the above single equations are the simplest bilinear equations of the hierarchy. To give a bilinear formulation for the other members of the hierarchy one has to add new independent time variables and new equations.[12–14]

Recently the bilinear formalism has received a far-reaching interpretation by the Kyoto school.[13] They have related several hierarchies of integrable bilinear equations to Kac–Moody algebras. An important ingredient in this approach is the use of an infinite number of time coordinates in a certain well-orchestrated manner (this has already appeared in textbooks, see Ref. 14). In this approach the most basic system is the KP hierarchy, whose single-equation member is the KP equation (15) above. Many other equations can be obtained from these basic hierarchies by certain reduction methods.[13,15,16]

As was mentioned above, any equation that can be written in the bilinear formalism has two-soliton solutions, but the situation is much more complicated even for three-soliton solutions. Ramani has studied[17] the integrability of various NEE's as mirrored by the Painlevé analysis and compared it with the existence of three-soliton solutions. He draws the conclusion that the Painlevé property and the existence of three-soliton solutions go hand in hand, suggesting the conjecture that the existence of three-soliton solutions implies complete integrability. An interesting new model is found in this process

$$(D_x{}^6 + D_x{}^3 D_t + kD_t{}^2) F\cdot F = 0\,. \tag{19}$$

It passes the Painlevé test precisely for $k = -\frac{1}{5}$, which is also the only value for which it has three-soliton solutions.

In this paper we present results of a search for bilinear equations of type (6), which have three-soliton solutions. The search extended up to polynomials $P(D_x,D_t)$ of total degree 8. Surprisingly enough one new equation was found already at degree 4. Some of the results generalize to higher dimensions. The extensive calculations were done with a computer, mostly using the symbol manipulation language REDUCE.

The paper is organized as follows: In the next section we show that all NEE's that can be put into the bilinear form (6) have two-soliton solutions, and after this derive the three-soliton condition (3SC). In Sec. III we discuss how the condition can be formulated in the language of algebraic geometry. The method of classification, which proceeds from monomials to homogeneous polynomials to general polynomials, is presented in Sec. IV. The main search is done in two dimensions, but the results are extended to higher dimensions in Sec. IV F.

II. PROPERTIES OF BILINEARIZABLE EQUATIONS

Hirota used the bilinear formalism to construct closed form multisoliton solutions for various systems. Most PDE's have traveling wave solutions but only in exceptional cases do they have solutions where these traveling waves scatter elastically, i.e., are true solitons. An important result is that *if the equation can be put in a bilinear form it will always have at least two-soliton solutions*,[3] as we will now show.

Let us consider a bilinear equation of the form (6). To get a single soliton solution we take for F the exponential ansatz

$$F = 1 + e^n, \quad n = px + \Omega t + m\,, \tag{20}$$

where p, Ω, and m are constant parameters. (For generalizations, see Refs. 18–20.) Note that F does not have a lump-type shape, but u defined by (3) or (8) does have. This F is a solution of (6), provided that the parameters p and Ω of the soliton are chosen so that they satisfy the *dispersion relation*

$$P(p,\Omega) = 0. \tag{21}$$

At this point we also get some mild conditions for the polynomial P: It must be even and without a constant term

$$P(D_x,D_t) = P(-D_x,-D_t), \quad P(0,0) = 0\,. \tag{22}$$

A two-soliton solution can always be constructed for (6). As an ansatz take

$$F = 1 + e^{n_1} + e^{n_2} + B_{12} e^{n_1+n_2}\,, \tag{23}$$

where

$$n_i = p_i x + \Omega_i t + m_i\,, \tag{24}$$

for each $i = 1,2$. This solves (6) if (21) holds for each pair (p_i,Ω_i) and if the new constant B_{12} is chosen to be

$$B_{12} = -P(p_1 - p_2,\Omega_1 - \Omega_2)/P(p_1 + p_2,\Omega_1 + \Omega_2)\,. \tag{25}$$

This method of constructing a two-soliton solution works for *all* nonlinear equations that can be cast in the bilinear form (6) with (22). However, when the ansatz (23) is extended to three or more solitons we get stringent conditions for the polynomial P.

For the general N-soliton solution Hirota starts with a generalization of (23) and writes F in the form[3]

$$F = \sum_{\mu=0,1} \exp\left[\sum_{i>j}^{(N)} A_{ij}\mu_i\mu_j + \sum_{i=1}^{N} \mu_i n_i\right], \tag{26}$$

where the n_i are given as before in (24). When (26) is substituted into (6) we obtain at first order in e^n the condition (21) for the constants p_i, Ω_i, $i = 1,\ldots,N$. The constants A_{ij} are determined at second order in e^n by the analog of (25)

$$\exp A_{ij} = -P(p_i - p_j,\Omega_i - \Omega_j)/P(p_i + p_j,\Omega_i + \Omega_j)\,. \tag{27}$$

At higher orders one obtains conditions of the type

$$S[P,n] \equiv \sum_{\sigma=\pm 1} P\left(\sum_{i=1}^{n} \sigma_i p_{k_i}, \sum_{i=1}^{n} \sigma_i \Omega_{k_i}\right) \times \prod_{i>j}^{(n)} P(\sigma_i p_{k_i} - \sigma_j p_{k_j}, \sigma_i \Omega_{k_i} - \sigma_j \Omega_{k_j}) \sigma_i \sigma_j = 0 , \tag{28}$$

for each $n = 1,...,N$, and $k_i \in \{1,...,N\}$ with $k_i > k_j$ for $i > j$, and for all p_k, Ω_k subject to (21). [Note that for $n = 1$ or 2 Eq. (28) is satisfied automatically.] Equation (28) is to be regarded as a condition on P rather than on the parameters p_k and Ω_k, therefore it is sufficient that the indices k_i also range from 1 to n, and k_i and k_j may in (28) be replaced by i and j, respectively. Equation (28) and the preceding calculations generalize immediately to a higher number of parameters used in multidimensional equations.

For a three-soliton solution one gets the first nontrivial conditions form (28) ($n = N = 3$), the three-soliton condition (3SC), which is the main subject of this paper.

The 3SC was studied numerically by Ito[21] for some specific cases. As a new result he found that a generalization of (13), namely

$$P \equiv D_x{}^3 D_t + a D_x{}^2 + b D_x D_t + c D_t{}^2 + d D_t D_y , \tag{29}$$

also satisfies (28).

Recently (28) has been studied in Ref. 22. In that paper a multitime approach was used with

$$n = \sum_{r=0}^{\infty} (-1)^r k^{2r+1} t_{2r+1} .$$

This choice is related to the KdV family, since in two dimensions it implies $p = k$, $\Omega = -k^3$, which is clearly a solution of the KdV dispersion equations $p^4 + p\Omega = 0$ [cf. (4) and (21)]. In this paper no such specific relation is assumed between p and Ω.

III. FORMULATION OF THE PROBLEM IN THE LANGUAGE OF ALGEBRAIC GEOMETRY

A. General discussion

According to the previous section the N-soliton condition has the following formulation.

F1: A bilinear equation $P(D_x, D_t)F \cdot F = 0$ has N-soliton solutions, if the polynomials $S[P,n](\mathbf{x},\mathbf{t})$ ($n = 1,...,N$) derived from $P(X,T)$ according to (28) vanish at points $(\mathbf{x},\mathbf{t})$ for which $P(x_i,t_i) = 0$ for all $i = 1,...,n$.

[For clarity we have changed the notation from (p_i,Ω_i) to (x_i,t_i), and also denoted $\mathbf{x} = (x_1,...,x_n)$, etc.] Problems of this type, relating the zero sets of various polynomials, are best formulated in the language of affine algebraic geometry. We will start by recalling some basic definitions.[23]

The ring of polynomials in the variables X and T over $\mathbb{C}$ will be denoted by $\mathbb{C}[X,T]$. The ideal generated by a polynomial $P(X,T)$ is given by $\langle P \rangle = \{PQ \,|\, Q \in \mathbb{C}[X,T]\}$. For the affine space we take $A = \mathbb{C}^2$ (where the vector space properties are ignored). A given $P \in \mathbb{C}[X,T]$ defines an affine manifold V_P in A by

$$V_P = \{(x,t) \in A \,|\, P(x,t) = 0\} . \tag{30}$$

In the present context the algebraic curve V_P will be called *dispersion manifold*. Instead of the polynomial P we may here take the ideal $\langle P \rangle$ generated by it, and define, in general,

$$V_I = \{(x,t) \in A \,|\, \forall p \in I,\ p(x,t) = 0\} . \tag{31}$$

Conversely, the polynomials that vanish on V_I form an ideal, $I(V_I)$. In general we have $I \subseteq I(V_I)$.

The previous definitions were given for one polynomial of two variables, but they generalize immediately to any finite number of polynomials in a finite number of variables. Let us next take $\mathbb{C}[\mathbf{X},\mathbf{T}] = \mathbb{C}[X_1,...,X_N, T_1,...,T_N]$, into which the polynomial $S[P,N]$ in the N-soliton condition belongs. The corresponding affine space is $\mathbb{C}^{2N}$. The dispersion manifold V_P (30) can be embedded into $\mathbb{C}^{2N}$ in N ways:

$$V_P{}^{(i)} = \{(x,t) \in \mathbb{C}^{2N} \,|\, P(x_i,t_i) = 0\} , \tag{32}$$

for $i = 1,...,N$. Let us also define $V_{P,N}$ by

$$V_{P,N} = \{(x,t) \in \mathbb{C}^{2N} \,|\, P(x_i,t_i) = 0,\ \forall\, i = 1,...,N\} = \bigcap_i V_P{}^{(i)} . \tag{33}$$

With these definitions we get a second formulation equivalent to F1:

F2: The polynomial P satisfies the N-soliton condition iff $S[P,n] \in I(V_{P,n})$, for $n = 1,...,N$.

It is important at this point to realize that the correspondence between the polynomial P and the ideal $I(V_{P,N})$ is not 1–1. So although the explicit form of the potential is needed to construct $S[P,N]$, only the zero set of P is of importance when we consider the ideal generated by $V_{P,N}$. To clarify this point we have to introduce one more definition. For an ideal I in the ring R its radical ideal $\sqrt{I}$ is defined by

$$\sqrt{I} = \{p \in R \,|\, \exists n \text{ s.t. } p^n \in I\} . \tag{34}$$

We observe (Ref. 23, p. 22) that $\sqrt{I} = I(V_I)$.

Thus for a given polynomial we must construct its radical ideal. Since the polynomial ring $\mathbb{C}[X,T]$ is a unique factorization domain, the polynomial $P(X,T)$ can be decomposed uniquely into irreducible factors as

$$P(X,T) = \text{const} \times \prod_j Q_j(X,T)^{n_j} , \tag{35}$$

where each Q_j is a monic (i.e., leading coeff. = 1) irreducible polynomial. The irreducible affine manifold $V(Q)$ corresponding to the irreducible polynomial Q is called an affine variety; $V(P) = \cup_j V(Q_j)$. [The overall constant in (35) can be omitted since it factors out in the definition of the dispersion manifold and in the N-soliton condition.]

It will be useful later to combine those factors that have the same multiplicity n_j, and write P as

$$P(X,T) = \prod_{i=1}^{s} P_i(X,T)^{n_i}, \text{ where } n_i > n_j \text{ for } i < j . \tag{36}$$

For later use we introduce also the notation H_i for the leading homogeneous part of P_i, while the leading monomial (having the highest power of X) of H_i is denoted by M_i.

Associated with P we define

$$\sqrt{P}(X,T) = \prod_j Q_j(X,T) = \prod_i P_i(X,T) . \tag{37}$$

Clearly $\sqrt{P}(x,t) = 0$ iff $P(x,t) = 0$, thus $V_P = V_{\sqrt{P}}$, in fact $I(V_P) = \langle \sqrt{P} \rangle = \sqrt{\langle P \rangle}$ (Ref. 23, p. 22).

For our final formulation we need the following.

Theorem:

$$I(V_{P,n}) = \left\{ \sum_{i=1}^{n} \sqrt{P(X_i,T_i)} K_{n,i}(\mathbf{X},\mathbf{T}) \,\middle|\, K_{n,i} \in \mathbb{C}[\mathbf{X},\mathbf{T}] \right\}.$$

Proof: As a consequence of Hilbert's Nullstellensatz we can write the rhs as

$$\sum_i I(V_P{}^{(i)}) = \sum_i I(\bigcup_j V_{Q_j}{}^{(i)}) = \sum_i \bigcap_j I(V_{Q_j}{}^{(i)})$$

while for the lhs we obtain

$$I(V_{P,n}) = I\left(\bigcap_i \bigcup_j V_{Q_j}{}^{(i)}\right) = \bigcap_{j_1} \cdots \bigcap_{j_n} I\left(\bigcap_i V_{Q_{j_i}}{}^{(i)}\right),$$

where we have used the property $I(\cup_k V_k) = \cap_k I(V_k)$. For the next steps we have to use the fact that the $V_Q{}^{(i)}$'s with different i's have polynomial conditions that depend on different sets of variables. Then $\cap_i V_{Q_{j_i}}{}^{(i)}$ can be interpreted as a Cartesian product of the affine varieties $V_{Q_{j_i}}$ and in such a case we have $I(V \times W) = \langle I(V) \cup I(W) \rangle$ (Ref. 24, p. 86). Thus if the $I(V^{(i)})$'s are interpreted as ideals in the common ring $\mathbb{C}[\mathbf{X},\mathbf{T}]$ we obtain

$$I\left(\bigcap_i V_{Q_{j_i}}{}^{(i)}\right) = \sum_i I(V_{Q_{j_i}}{}^{(i)}).$$

Again, if the variables appearing in the generators of I are different from those appearing in the generators of J and K, then we have the distribution law $I + J \cap K = (I + J) \cap (I + K)$. Using it repeatedly we conclude the proof. ■

With this result we can finally write the N-soliton condition in a computable way as follows.

F3: The polynomial $P(X,T)$ passes Hirota's N-soliton condition iff we can write

$$S[P,n] = \sum_{i=1}^{n} \sqrt{P(X_i,T_i)} K_{n,i}(\mathbf{X},\mathbf{T}), \tag{38}$$

for $n = 1,\ldots,N$ with some polynomials $K_{n,i} \in \mathbb{C}[\mathbf{X},\mathbf{T}]$. Note that the original polynomial P enters in the left-hand side, but only its radical on the right-hand side.

In the special case of three-soliton solutions we get just one extra condition, namely (38) for $n = 3$, i.e.,

$$S[P,3] = \sqrt{P(X_1,T_1)} A(\mathbf{X},\mathbf{T}) + \sqrt{P(X_2,T_2)} B(\mathbf{X},\mathbf{T}) + \sqrt{P(X_3,T_3)} C(\mathbf{X},\mathbf{T}). \tag{39}$$

There is another, perhaps more intuitive, way to arrive to (39). Let us choose three points $(a^i,b^i) \in V_P$, $i = 1,2,3$, corresponding to the three solitons. We embed them in $\mathbb{C}^6$ as $(\mathbf{a},\mathbf{b}) = (a^1,a^2,a^3,b^1,b^2,b^3) \in V_{P,3}$. There will then be some j_i so that [cf. (32), (35)]

$$(\mathbf{a},\mathbf{b}) \in \bigcap_i V_{Q_{j_i}}{}^{(i)} \equiv \bigcap_i V(j_i).$$

As we let each (a^i,b^i) vary independently over V_P we see that it is enough if $S[P,3]$ vanishes in $V(j_1) \cap V(j_2) \cap V(j_3)$ for all possible choices of the three j_i's. But the union over these choices yields nothing but $V_{P,3}$ as defined in (33), so the previous result is again obtained.

B. Interpretation for the computer

To test whether $S[P,3]$ can be written in the form (39) one could, in principle, substitute a sufficiently general ansatz for the polynomials A, B, and C and try to solve for the unknown coefficients. However, $S[P,3]$ is so complicated even for rather simple polynomials that this approach is, in practice, impossible. What was done instead was to interpret Eq. (39) using a rewrite rule. For each i we took the leading monomial $\sqrt{M(X_i,T_i)}$ of $\sqrt{P(X_i,T_i)}$ and replaced it everywhere in $S[P,3]$ by the expression $\sqrt{M(X_i,T_i)} - \sqrt{P(X_i,T_i)}$, until no factors of $\sqrt{M(X_i,T_i)}$ appeared in the expression, or it vanished. For example, in the KdV case it means replacing X_i^4 by $-X_iT_i$ for each i wherever a factor of X_i^4 can be extracted. Evidently, $S[P,3]$ vanishes in this process if and only if it can be written as in (39). Of course the substitution must usually be made several times until all factors of $\sqrt{M(X_i,T_i)}$ disappear. In REDUCE this is accomplished using a LET statement.[25]

Most of the computations were done using computer algebra systems. The simplest problems were solved using muMATH in a PC computer, for more complicated ones we used REDUCE, first in DEC-20 and later in IBM 3081.

IV. THE METHOD OF CLASSIFICATION

A. Preliminary remarks

It is clear that the property of passing 3SC is invariant under any nonsingular linear change of coordinates. It is useful to eliminate part of this freedom by fixing the coordinate system.

The coordinate system is fixed in the following manner: Let us take the polynomial factor P_1 (which has the maximum multiplicity n_1) and in it the homogeneous polynomial with the highest degree H_1. Now H_1 factors into linear factors and of these we choose the one with the highest multiplicity, let us denote it by $L_1 = aX + bT$. If this monomial has other factors differing from L_1 we take the one with next highest power as $L_2 = cX + dT$. If H_1 is just a power of L_1 we check the leading monomial of P_2 (which has the next highest multiplicity), and so on. If all the H_k's are powers of L_1 we continue with the next to leading monomials, etc. until another linear factor is found, or $P = P(L_1)$ and the system is one dimensional. If two factors are found we make the transformation to new coordinates defined by

$$X_{\text{new}} = L_1, \quad T_{\text{new}} = L_2. \tag{40}$$

This choice of coordinates will greatly simplify the classification process. It still leaves the possibility of scaling T, which will be used later.

As the previous discussion shows we must in the various steps of the classification process keep account of the multiplicities of the original polynomial. To keep track of this we will use square brackets to indicate the original grouping of polynomials given in (36). We write

$$P_h = \prod_i [H_i]^{n_i}, \quad \sqrt{P_h} = \prod_i [H_i], \tag{41}$$

and similarly for P_m and $\sqrt{P_m}$. Note that we mean $[\sqrt{P}]_h$, which respects the previous factorization, and not $\sqrt{[P_h]}$.

One essential component in the bilinear treatment of the present case is that $P(X,T)$ is an even polynomial without a constant term (22). We assume here that when the invariance under $X\to -X$, $T\to -T$ is applied to the factorized form (36) it implies a fixed parity for all factors, i.e., that $P_i(-X,-T)=\pm P_i(X,T)$ for each i.

B. Reduction from P to a homogeneous to a monomial problem

In the condition for $S[P,3]$ (39) it is of course necessary that it holds for the highest-order homogeneous part by itself. This is clear from the equation, where the highest degree terms can be isolated, but it holds equally well using rewrite rules: we just replace $[\sqrt{P}]_m(X_i,T_i)$ everywhere in $S[P_h,3]$ by the expression $[\sqrt{P}]_m(X_i,T_i)-[\sqrt{P}]_h(X_i,T_i)$.

We take one more step: If the homogeneous part is to vanish we must assume that the highest degree (in X_i's) monomial part in the equation vanishes by itself. In terms of rewrite rules this means that $S[P_m,3]$ should vanish after substituting zero for each occurrence of $[\sqrt{P}]_m$.

The first step in the classification is, therefore, to discuss the monomials for which the three-soliton condition is satisfied for various relevant $[\sqrt{P}]_m$.

C. Monomials

To start we observe that monomials in one variable always pass the three-soliton test. We may assume that after the possible change of coordinates described in Sec. IV A we have $P_m=X^M$ and $[\sqrt{P}]_m=X^K$, where $M\geqslant K$. The degree of $S[X^M,3]$ is $4M$ and so in each monomial in $S[X^M,3]$ at least one of the three X_i's will have a degree greater than M, therefore in each term a factor of X_i^K can be extracted for some i and thus expansion (39) is valid.

Monomials in two variables are discussed in detail in Appendix A. To summarize the results we introduce the auxiliary function μ by

$$\mu(k)=[(k+2)/4]+[(k+3)/4], \tag{42}$$

where the square brackets denote the integer part. The results can now be stated as follows: Let

$$P_m=X^MT^N,\quad [\sqrt{P}]_m=X^KT^L,$$
$$M+N\ \text{ even},\quad M\geqslant K>0,\quad N\geqslant L>0.$$

Necessary conditions for P_m to pass the three-soliton test are the following.

(1) If M is odd and $K=1$, then $L\leqslant\mu(N-1)+3$, or if $L=1$, then $K\leqslant\mu(M-1)+3$.

(2) If M is even and $N=L=2$, then $K\leqslant 2$, or if $M=K=2$, then $L\leqslant 2$.

(3) In all other cases $K\leqslant\mu(M)$ and $L\leqslant\mu(N)$.

In Appendix A these conditions were shown to be necessary, but they also appear to be sufficient. To be sure we checked them for $N+M<12$ by computer.

With these results we can start to construct Tables I–III. In the first column we give the type of the polynomial, (M,N). According to the choice of X and T in Sec. IV A the variable with highest multiplicity is X. Usually we have also $M\geqslant N$, and if $M<N$ we give the type as (N,M) and remind of this reversal by a letter R in the first column.

For the second column in the tables we consider the products

$$\prod_i [X^{r_i}T^{s_i}]^{n_i}, \tag{43}$$

for which

$$\sum_i r_in_i=M,\quad \sum_i r_i=K,\quad \sum_i s_in_i=N,\quad \sum_i s_i=L, \tag{44}$$

TABLE I. The classification steps for polynomials of degree 4.

Type	Leading monomial	Possible homogeneous generalization	Accepted homog. generalization	Possible generalizations	Accepted final result	Comments
(4.0)						
	$[X]^4$		$[X]^4$		$[X]^4$	1 dim
	$[X]^2[X^2]$		$[X]^2[X^2]$	$[X]^2[X^2-1]$	$[X]^2[X^2-1]$	1 dim
	$[X^4]$		$[X^4]$	$[X^4+aX^2+bXT+cT^2]$	$[X^4+aX^2+bXT+cT^2]$	(I A)
(3.1)						
	$[X]^3[T]$		$[X]^3[T]$		$[X]^3[T]$	$o(3,1)$
	$[X]^2[XT]$	$[X]^2[(X+aT)T]$	$[X]^2[XT]$	$[X]^2[XT+1]$	$[X]^2[XT+1]$	see below
			$[X]^2[(X+T)T]$	$[X]^2[(X+T)T+R_0]$	$[X]^2[(X+T)T]$	$o(2,1,1)$
	$[X^3T]$	$[XT(X^2+\cdots)]$	$[XT(X^2+\cdots)]$	$[XT(X^2+\cdots)+R_2]$	$[XT(X^2+aXT+T^2)]$	$o(1,1,1,1)$
					$[X^3T+aX^2+bXT+cT^2]$	(I B)
					$[XT(X^2+\sqrt{3}XT+T^2)$ $+aX^2+bXT+cT^2]$	(I C)
(2.2)						
	$[XT]^2$		$[XT]^2$		$[XT]^2$	$o(2,2)$
	$[X]^2[T^2]$		$[X]^2[T^2]$	$[X]^2[T^2-1]$	$\cdots$	
	$[X^2T^2]$		$[X^2T^2]$	$[X^2T^2+R_2]$	$\cdots$	

TABLE II. The classification steps for polynomials of degree 6.

Type	Leading monomial	Possible homogeneous generalization	Accepted homog. generalization	Possible generalizations	Accepted final result	Comments
(6.0)						
	$[X]^6$		$[X]^6$		$[X]^6$	$o(6)$
	$[X]^4[X^2]$		$[X]^4[X^2]$	$[X]^4[X^2-1]$	$[X]^4[X^2-1]$	1 dim
	$[X]^3[X^3]$		$[X]^3[X^3]$	$[X]^3[X^3+R_1]$	$\cdots$	
	$[X]^2[X^4]$		$[X]^2[X^4]$	$[X]^2[X^4+R_2+R_0]$	$[X]^2[X^4+aX^2+1]$	1 dim
	$[X^3]^2$		$[X^3]^2$	$[X^3+R_1]^2$	$\cdots$	
	$[X^6]$		$[X^6]$	$[X^6+R_4+R_2]$	$[X^6+aX^4+XT]$	(I D 1)
					$[X^6+5X^3T-5T^2+aX^2+bXT]$	(I D 2)
(5.1)						
	$[X]^5[T]$		$[X]^5[T]$		$[X]^5[T]$	$o(5,1)$
	$[X]^4[XT]$	$[X]^4[(X+aT)T]$	$[X]^4[XT]$	$[X]^4[XT+1]$	$\cdots$	
			$[X]^4[(X+T)T]$	$[X]^4[(X+T)T+a]$	$[X]^4[(X+T)T]$	$o(4,1,1)$
	$[X^2]^2[XT]$	$[X^2]^2[(X+aT)T]$	$[X^2]^2[XT]$	$[X^2-1]^2[XT]$	$[X^2-1]^2[XT]$	$p(2;1,1)$
			$[X^2]^2[(X+T)T]$	$[X^2-1]^2[(X+T)T]$	$\cdots$	
	$[X]^3[X^2T]$	$[X]^3[(X^2+\cdots)T]$	$[X]^3[X^2T]$	$[X]^3[X^2T+R_1]$	$[X]^3[(X^2-1)T]$	$p(1;3,1)$
			$[X]^3[XT(X+T)]$	$[X]^3[XT(X+T)+R_1]$	$\cdots$	
	$[X]^2[X^3T]$	$[X]^2[(X^3+\cdots)T]$	$[X]^2[X^3T]$	$[X]^2[X^3T+R_2+R_0]$	$\cdots$	
	$[X^5T]$	$[(X^4+\cdots)XT]$	$[X^5T]$	$[X^5T+R_4+R_2]$	$\cdots$	
(4.2)						
	$[X]^4[T]^2$		$[X]^4[T]^2$		$[X]^4[T]^2$	$o(4,2)$
	$[X]^4[T^2]$		$[X]^4[T^2]$	$[X]^4[T^2-1]$	$\cdots$	
	$[X^2T]^2$	$[XT(X+aT)]^2$	$[X^2T]^2$	$[X^2T+R_1]^2$	$\cdots$	
	$[X]^3[T]^2[X]$	$[X]^3[T]^2[X+aT]$	$[X]^3[T]^2[X]$	$\cdots$	$\cdots$	
			$[X]^3[T]^2[X+T]$	$[X]^3[T]^2[X+T]$	$[X]^3[T]^2[X+T]$	$o(3,2,1)$
	$[X]^3[XT^2]$	$[X]^3[(X+aT)T^2]$	$[X]^3[XT^2]$	$[X]^3[XT^2+R_1]$	$\cdots$	
(3.3)						
	$[XT]^3$		$[XT]^3$		$[XT]^3$	$o(3,3)$
	$[X]^3[T^3]$		$[X]^3[T^3]$	$[X]^3[T^3+R_1]$	$[X]^3[(T^2-1)T]$	$p(1;1,3)$
	$[XT]^2[XT]$	$[XT]^2[(X+aT)T]$	$[XT]^2[XT]$	$[XT]^2[XT+1]$	$\cdots$	
				$[XT+1]^2[XT]$	$\cdots$	

with M, K, N, and L satisfying the conditions (1)–(3) above.

It is not necessary, however, to take all of the monomials, for some of them cannot possibly lead to an acceptable final result. This is mainly because they will eventually conflict with the definition of $\sqrt{P}$, the choice of the coordinates, or the condition $P(0,0)=0$. The following additional conditions are easily shown to be necessary.

(1) Let k be such that $s_i=0$ for all $i<k$. Then there can be at most one $j<k$ for which $r_j=1$.

(2) If $s_1\neq 0$ then $r_1\geqslant s_1$.

(3) At least one r_i or s_i must be $\neq 2$.

TABLE III. The classification steps for polynomials of degree 8.

Type	Leading monomial	Possible homogeneous generalization	Accepted homog. generalization	Possible generalizations	Accepted final result	Comments
(8.0)						
	$[X]^8$		$[X]^8$		$[X]^8$	$o(8)$
	$[X^2]^3[X]^2$		$[X^2]^3[X]^2$	$[X^2-1]^3[X]^2$	$[X^2-1]^3[X]^2$	1 dim
	$[X]^4[X^2]^2$		$[X]^4[X^2]^2$	$[X]^4[X^2-1]^2$	$[X]^4[X^2-1]^2$	1 dim
	$[X^4]^2$		$[X^4]^2$	$[X^4+R_2]^2$	$\cdots$	
	$[X]^6[X^2]$		$[X]^6[X^2]$	$[X]^6[X^2-1]$	$[X]^6[X^2-1]$	1 dim
	$[X^3]^2[X^2]$		$[X^3]^2[X^2]$	$[X^3+R_1]^2[X^2-1]$	$\cdots$	
	$[X]^5[X^3]$		$[X]^5[X^3]$	$[X]^5[X^3+R_1]$	$\cdots$	
	$[X]^4[X^4]$		$[X]^4[X^4]$	$[X]^4[X^4+R_2+R_0]$	$[X]^4[X^4+aX^2+1]$	1 dim
	$[X^2]^2[X^4]$		$[X^2]^2[X^4]$	$[X^2-1]^2[X^4+R_2]$	$\cdots$	
	$[X]^3[X^5]$		$[X]^3[X^5]$	$[X]^3[X^5+R_3+R_1]$	$\cdots$	
	$[X]^2[X^6]$		$[X]^2[X^6]$	$[X]^2[X^6+R_4+R_2+R_0]$	$[X]^2[X^6+2aX^4+a^2X^2+1]$	1 dim
	$[X^8]$		$[X^8]$	$[X^8+R_6+R_4+R_2]$	$\cdots$	

TABLE III. (*Continued.*)

Type	Leading monomial	Possible homogeneous generalization	Accepted homog. generalization	Possible generalizations	Accepted final result	Comments
(7.1)						
	$[X]^7[T]$		$[X]^7[T]$		$[X]^7[T]$	$o(7,1)$
	$[X]^3[X^2]^2[T]$		$[X]^3[X^2]^2[T]$	$[X]^3[X^2-1]^2[T]$	$[X]^3[X^2-1]^2[T]$	$p(2;3,1)$
	$[X]^6[XT]$	$[X]^6[(X+aT)T]$	$[X]^6[XT]$	$[X]^6[XT+1]$	⋯	
			$[X]^6[(X+T)T]$	$[X]^6[(X+T)T+R_0]$	$[X]^6[(X+T)T]$	$o(6,1,1)$
	$[X^2]^3[XT]$	$[X^2]^3[(X+aT)T]$	$[X^2]^3[XT]$	$[X^2-1]^3[XT]$	$[X^2-1]^3[XT]$	$p(3;1,1)$
			$[X^2]^2[(X+T)T]$	$[X^2-1]^3[(X+T)T]$	⋯	
	$[X^3]^2[XT]$	$[X^3]^2[(X+aT)T]$	$[X^3]^2[XT]$	$[X^3+R_1]^2[XT+R_0]$	⋯	
	$[X]^5[X^2T]$	$[X]^5[XT(X+aT)]$	$[X]^5[X^2T]$	$[X]^5[X^2T+R_1]$	$[X]^5[(X^2-1)T]$	$p(1;5,1)$
			$[X]^5[XT(X+T)]$	$[X]^5[XT(X+T)+R_1]$	⋯	
	$[X]^4[X^3T]$	$[X]^4[XT(X^2+\cdots)]$	$[X]^4[X^3T]$	$[X]^4[XT+R_2+R_0]$	⋯	
	$[X^2]^2[X^3T]$	$[X^2]^2[XT(X^2+\cdots)]$	$[X^2]^2[X^3T]$	$[X^2-1]^2[X^3T+R_2]$	⋯	
	$[X]^3[X^4T]$	$[X]^3[XT(X^3+\cdots)]$	$[X]^3[X^4T]$	$[X]^3[X^4T+R_3+R_1]$	⋯	
	$[X]^2[X^5T]$	$[X]^2[XT(X^4+\cdots)]$	$[X]^2[X^5T]$	$[X]^2[X^5T+R_4+R_2+R_0]$	⋯	
	$[X^7T]$	$[XT(X^6+\cdots)]$	$[X^7T]$	$[X^7T+R_6+R_4+R_2]$	⋯	
(6.2)						
	$[X]^6[T]^2$		$[X]^6[T]^2$		$[X]^6[T]^2$	$o(6,2)$
	$[X]^6[T^2]$		$[X]^6[T^2]$	$[X]^6[T^2-1]$	⋯	
	$[X^2]^3[T]^2$		$[X^2]^3[T]^2$	$[X^2-1]^3[T]^2$	⋯	
	$[X]^4[XT]^2$	$[X]^4[(X+aT)T]^2$	$[X]^4[XT]^2$	$[X]^4[XT+1]^2$	⋯	
	$[X^3T]^2$	$[XT(X^2+\cdots)]^2$	$[X^3T]^2$	$[X^3T+R_2]^2$	⋯	
	$[X]^5[T]^2[X]$	$[X]^5[T]^2[X+aT]$	$[X]^5[T]^2[X]$	⋯	⋯	
			$[X]^5[T]^2[X+T]$		$[X]^5[T]^2[X+T]$	$o(5,2,1)$
	$[X]^5[XT^2]$	$[X]^5[(X+aT)T^2]$	$[X]^5[XT^2]$	$[X]^5[XT^2+R_1]$	⋯	
	$[X]^3[XT]^2[X]$	$[X]^3[(X+aT)T]^2[X+bT]$	$[X]^3[XT]^2[X]$	⋯	⋯	
	$[X]^4[T]^2[X^2]$	$[X]^4[T]^2[X^2+\cdots]$	$[X]^4[T]^2[X^2]$	$[X]^4[T]^2[X^2-1]$	⋯	
	$[X^2T]^2[X^2]$	$[XT(X+aT)]^2[X^2+\cdots]$	$[X^2T]^2[X^2]$	$[X^2T+R_1]^2[X^2-1]$	⋯	
	$[X]^3[T]^2[X^3]$	$[X]^3[T]^2[X^3+\cdots]$	$[X]^3[T]^2[X^3]$	$[X]^3[T]^2[X^3+R_1]$	⋯	
(5.3)						
	$[X]^5[T]^3$		$[X]^5[T]^3$		$[X]^5[T]^3$	$o(5,3)$
	$[X]^5[T^3]$		$[X]^5[T^3]$	$[X]^5[T^3+R_1]$	$[X]^5[T(T^2-1)]$	$p(1;1,5)$
	$[XT]^3[X]^2$	$[XT]^3[X+aT]^2$	$[XT]^3[X]^2$	$[XT+1]^3[X]^2$	⋯	
			$[XT]^3[X+T]^2$		$[XT]^3[X+T]^2$	$o(3,3,2)$
	$[X]^3[XT]^2[T]$	$[X]^3[(X+aT)T]^2[T]$	$[X]^3[XT]^2[T]$	$[X]^3[XT+1]^2[T]$	⋯	
	$[X]^4[T]^3[X]$	$[X]^4[T]^3[X+aT]$	$[X]^4[T]^3[X]$	⋯	⋯	
			$[X]^4[T]^3[X+T]$		$[X]^4[T]^3[X+T]$	$o(4,3,1)$
	$[X]^4[T]^2[XT]$	$[X]^4[T]^2[(X+aT)T]$	$[X]^4[T]^2[XT]$	$[X]^4[T]^2[XT+1]$	⋯	
	$[X^2T]^2[XT]$	$[XT(X+aT)]^2[(X+bT)T]$	$[X^2T]^2[XT]$	$[X^2T+R_1]^2[XT+R_0]$	⋯	
	$[XT]^3[X^2]$	$[XT]^3[X^2+\cdots]$	$[XT]^3[X^2]$	$[XT]^3[X^2-1]$	$[XT]^3[X^2-1]$	$p(1;3,3)$
			$[XT]^3[X(X+T)]$	$[XT+1]^3[X(X+T)]$	⋯	
				$[XT]^3[X(X+T)+1]$	⋯	
	$[X]^3[T]^2[X^2T]$	$[X]^3[T]^2[(X^2+\cdots)T]$	$[X]^3[T]^2[X^2T]$	$[X]^3[T]^2[X^2T+R_1]$	⋯	
R	$[X]^3[T^2]^2[T]$		$[X]^3[T^2]^2[T]$	$[X]^3[T^2-1]^2[T]$	$[X]^3[T^2-1]^2[T]$	$p(2;1,3)$
R	$[X]^3[T]^2[T^3]$		$[X]^3[T]^2[T^3]$	$[X]^3[T]^2[T^3+R_1]$	⋯	
R	$[X]^3[T^5]$		$[X]^3[T^5]$	$[X]^3[T^5+R_3+R_1]$	⋯	
(4.4)						
	$[XT]^4$		$[XT]^4$		$[XT]^4$	$o(4,4)$
	$[X]^4[T^2]^2$		$[X]^4[T^2]^2$	$[X]^4[T^2-1]^2$	⋯	
	$[X^2T^2]^2$		$[X^2T^2]^2$	$[X^2T^2+R_2]^2$	⋯	
	$[X]^3[T^2]^2[X]$	$[X]^3[T^2]^2[X+aT]$	$[X]^3[T^2]^2[X]$	⋯	⋯	
			$[X]^3[T^2]^2[X+T]$	$[X]^3[T^2-1]^2[X+T]$	⋯	
	$[XT]^3[XT]$	$[XT]^3[(X+aT)T]$	$[XT]^3[XT]$	$[XT+1]^3[XT]$	⋯	
				$[XT]^3[XT+1]$	⋯	
			$[XT]^3[(X+T)T]$	$[XT+1]^3[(X+T)T]$	⋯	
				$[XT]^3[(X+T)T+1]$	⋯	

The second column in Tables I–III can now be constructed.

D. Homogeneous polynomials

The next step is to reconstruct the most general homogeneous potential from the given monomials. Recalling again how the coordinate T was chosen we get certain restrictions in the possible generalizations, as above.

(4) Assume that k is defined as in (1) above, then each power of X for $j<k$ must stay monomial.

(5) If $s_1 \neq 0$ then s_1 powers of X must stay monomial.

With these rules we can write column 3 on Tables I–III. If no homogeneous generalizations were possible column 3 was left empty and the result of column 2 transferred directly to column 4.

All polynomials in column 3 were tested by computer whether they fulfilled 3SC. The positive results are given in column 4. We observe that arbitrary homogeneous polynomials of degree 4 are allowed, but for degree >4 one can only have a factor $(X+aT)$ in addition to the X and T factors we started with. In column 4 we have then used the freedom to scale T to $a=1$ or 0, and split the case into two subcases.

E. Final results in two dimensions

In column 5 we have written the most general nonhomogeneous polynomial as extended from the homogeneous polynomial in column 4, subject to the usual conditions that the generalization must be even, have no constant term, and will not conflict with the definition of $\sqrt{P}$. (For those cases that are eliminated by the last condition or which do not pass the 3SC we use three dots in the subsequent columns.) The notation R_i refers to an arbitrary homogeneous polynomial of degree i.

In column 6 we have as the result all those polynomials that pass the three-soliton test. The results can be divided into the following groups: (I) models with truly nonlinear dispersion manifold; and (II) models whose two-dimensional dispersion manifold consists of lines.

(I A) $X^4+aX^2+bXT+cT^2$. This is a combination of KdV and Boussinesq equations, for we have not yet used the freedom of choosing a new T variable. If $c=0$ we take $T_{\text{new}}=aX+bT$ and get KdV (4), while in the opposite case we first of all scale T so that $c=-1$, then take $T_{\text{new}}=T+\frac{1}{2}bX$, and finally scale X to obtain (9).

(I B) $X^3T+aX^2+bXT+cT^2$. This is a generalization of the shallow water wave equation (13), which is obtained after scaling for $a=0$. It is included as a special case $(d=0)$ in Ito's equation (29). The case $b=c=0$ appears as a separate item in the table because it has a different radical ideal.

(I C) $XT(X^2+\sqrt{3}XT+T^2)+aX^2+bXT+cT^2$. This is a new result. It is symmetric in X and T, a property not shared by any other nonhomogeneous bilinear equation of type (6). The leading polynomial can be transformed to many other forms, e.g., $X^4+6X^2T^2-3T^4$, but we prefer the canonical form. The leading fourth-order polynomial has an interesting property: If one chooses two factors from an arbitrary fourth-order homogeneous polynomial in X and T and redefines them as X and T then the remaining quadratic part of the polynomial will usually depend on the particular factors chosen. However, the above polynomial is one of the two, for which such redefinitions have no effect. Perhaps this high degree of symmetry is essential for a leading part that is not a mere power.

(I D1) X^6+aX^4+XT. This is a generalization of the Sawada–Kotera equation (11) which is obtained for $a=0$.

(I D2) $X^6+5X^3T+aX^2+bXT-5T^2$. This is a generalization of Ramani's equation (19), which is obtained for $a=b=0$ after scaling. Note the interesting feature that coefficients of different degree terms are related.

(II A) Several one-dimensional polynomials pass 3SC. At lower degrees the polynomial can be completely arbitrary, but at higher degrees we get conditions on the coefficients. Conditions are first obtained at degree 8: We find that the general polynomial $[X]^2[X^6+aX^4+bX^2+1]$ passes the three-soliton test only if $b=a^2/4$. This one case is not yet enough to determine the pattern and we will return to this subject in a later publication. One-dimensional bilinear equations are perhaps not relevant from the point of view of NEE's, but they should not be ignored because they may tell us something about the structure.

(II B) $p(N;M,P)=[X^2-1]^N X^M T^P$. At least for $2N+M+P<9$ this is acceptable if M and P are odd, which we conjecture to be sufficient for arbitrary degree.

(II C1) $o(M,N)=X^M T^N$. This is acceptable for any M and N.

(II C2) $o(M,N,P)=X^M T^N (X+T)^P$. This works whenever two of the indices M, N, P are odd.

(II D) $o(1,1,1,1)=XT(X+aT)(X+bT)$.

The notation $o(M,N,\ldots)$ is used above when the dispersion manifold consists of lines going through the origin, while for $p(N;M,P)$ it consists of three parallel lines and a fourth line intersecting them.

F. Extensions to higher dimensions

Let us finally discuss how some of the above results can be extended to higher dimensions. Our main tool in doing this is the observation that any higher-dimensional model must still pass the three-soliton test when it is projected to lower dimensions, i.e., if $P(D_x,D_t,D_y)$ is acceptable then so is $P(D_x,D_t,aD_x+bD_t)$ for *any* a and b. (This is because the condition is more stringent when the variable Y must be kept separate from the others.) This observation implies that we need only consider those models in the table that have enough arbitrariness.

(I A) In principle we should now test $X^4+aX^2+bXT+cT^2+dXY+eTY+fY^2$, but the freedom of redefining the T and Y coordinates can be used to simplify the situation.

(1) Let us first assume that $f\neq 0$, and scale Y so that $f=1$. By the transformation $Y\to Y+\alpha X+\beta T$ we can put $d=e=0$. If $b=c=0$, we get back to a two-dimensional model. If $c=0$, $b\neq 0$ we redefine T and scale so that the quadratic part has the conventional KP form $-4XT+3Y^2$, which passes the test. If $c\neq 0$ we scale T so that $c=-1$ and translate the quadratic part to $-T^2+aX^2$

$+ Y^2$. This, however, does not pass the three-soliton test.

(2) If $f=0$ we may by $T \leftrightarrow Y$ reflection assume that $c=0$ as well. Then redefining T we get either $X^4+X^2+Y(dX+eT)$ or $X^4+XT+Y(dX+eT)$. They pass the test only for $e=0$, which in each case can be reduced to two dimensions.

Since Y^2 was an accepted additional term we may ask next if an extension to four dimensions is possible. Using the same technique as above for reductions $Z=\alpha X+\beta T+\gamma Y$ one can show that the possible additional terms can either be absorbed or lead to one of the nonallowed extensions of the previous paragraph.

(I B) For this model we do not have the freedom to redefine T as in the previous case. First we checked the Y^2 extension and found that is not acceptable. For $aX^2+bXT+cT^2+dXY+eTY$ we found the condition $d=0$. We may then assume that $e=1$ and redefine Y so that $b=c=0$. Any higher-dimensional generalization must then also be of type XZ which can be eliminated by redefining Y. Thus our final result is X^3T+aX^2+TY. The additional aX^2 term was included in Ref. 21, but it is still open whether it can be obtained from some hierarchy by reduction methods of Refs. 13, 15, and 16. In any case if the final result is to be weighted homogeneous both T and X cannot have positive weight.

(I C) This model does not allow extensions to higher dimensions.

(I D) For (I D1) any extension would lead also to a generalization of the original two-dimensional model and are therefore excluded. For (I D2) one needs to consider only the additional term YX and it is found to be acceptable. Then we can redefine Y so that the model is finally $X^6+5X^3T-5T^2+XY$. It is the first equation of the BKP hierarchy,[13] and combines (I D1) and (I D2): with $Y \to aX+bT$ we obtain (I D2) while $T \to X$, $Y \to T$ yields (I D1).

(II A), (II B), and (II C1) do not allow generalizations to higher dimensions.

(II C2) In Appendix B we have derived for the three-dimensional extension of $o(M,N,P)=X^MT^NY^P$ the necessary condition that two of the indices M, N, and P must be odd. Since here $K=L=Q=1$ it is also sufficient. This agrees with the above two-dimensional discussion, and combines (II C1) and (II C2).

(II D) The only model with enough arbitrariness to be a candidate for a four-dimensional model is $o(1,1,1,1)$. Indeed, we find that $P=XTYZ$ passes the three-soliton test.

V. CONCLUSIONS

The full results are summarized in Table IV. We note that all the models of the first type with the exception of (I C) have been known previously. They can be obtained from certain KP hierarchies following the ideas of Ref. 13 [the aX^2 term in (I B) is still open]. Many other special cases can be obtained from these by projection or reduction.

The polynomial (I C) is a new result and interesting in its symmetrical treatment of the X and T variables. It seems unlikely that it can be obtained from the known hierarchies, because of its novel leading part. It is still open whether or not it is completely integrable, but in any case it passes the three-soliton test.

TABLE IV. Summary of the results of the search. The first group of models are truly nonlinear, (I C) being a new result. The second group of models have a linear dispersion manifold. These apparently infinite sequences are also new results.

(I A)	$X^4-4XT+3Y^2$
(I B)	X^3T+aX^2+TY
(I C)	$XT(X^2+\sqrt{3}XT+T^2)+aX^2+bXT+cT^2$
(I D)	$X^6+5X^3T-5T^2+XY$
(II A)	One-dimensional models, including $X^2[X^2(X^2+a)^2+1]$
(II B)	$[X^2-1]^NX^MT^P$, if M and P are odd
(II C)	$X^MT^NY^P$, if two exponents are odd
(II D)	$XTYZ$

The remaining models are special by having linear dispersion manifolds. Their complete integrability is not known, and it is not clear whether they can be obtained from the known hierarchies, or whether a new treatment is needed. It is also important to note that we obtained *infinite sequences* of models. As opposed to the hierarchies known before, which might be labeled "vertical" hierarchies, we have here "horizontal" hierarchies. An interesting question is whether vertical hierarchies can be built on top of them.

In this work we have assumed that the bilinear equation is of the type (6). Searches like this will be conducted for other types of equations in the future.

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APPENDIX A: MONOMIALS IN TWO VARIABLES

Here we will derive the necessary conditions for monomials in two variables to pass the three-soliton test. In general we have $P_m=X^MT^N$, $[\sqrt{P}]_m=X^KT^L$, $M+N$ even, $M \geqslant K$, $N \geqslant L$, and the three-soliton condition reads as follows: $S[X^MT^N,3]$ must vanish when the rewrite rule $X^KT^L \to 0$ is used. Here the constants K and L are carryovers from the initial factorization, since $\sqrt{(X^NT^M)}=XT$ if M, $N>0$. Let us introduce the notation

$$X_{ij}=(X_i^3X_j-X_iX_j^3)\sigma_i\sigma_j\,, \tag{A1}$$

and similarly for T_{ij}. Then $S[X^MT^N,3]$ can be conveniently written as

$$S[X^MT^N,3] = \sum_{\sigma}[X_{12}+X_{23}+X_{31}]^M[T_{12}+T_{23}+T_{31}]^N\,. \tag{A2}$$

Since the rewrite rule does not connect different monomials obtained after (A2) is expanded, they must all vanish independently. We will now consider some specially chosen groups of terms and in this way derive necessary conditions for K and L. The discussion will be divided into several subcases. Since X and T appear on the same footing the results obtained for M and K have their obvious analogs for N and L.

(a) N, M even. Let us consider the group of terms with the maximum power $3N$ of X_3 and no T_3. It is given by

$$\sum_\sigma X_3{}^{3M}(\sigma_1 X_1 - \sigma_2 X_2)^M (T_1{}^3 T_2 - T_1 T_2{}^3)^N . \tag{A3}$$

In this expression the powers of T_1 and T_2 are higher than K, so all terms that have sufficiently high powers of X_1 or X_2 will vanish. Let us therefore take the terms where these appear with minimum powers.

(a1) $M = 4m$, $m > 0$. The middle term in the expansion of $(\sigma_1 X_1 - \sigma_2 X_2)^M$ yields a term proportional to $X_3{}^{3M}(X_1 X_2)^{2m}(T_1{}^3 T_2 - T_1 T_2{}^3)^N$ and this vanishes only if $K \leqslant 2m$.

(a2) $M = 4m + 2$. Now the middle terms will have a $\sigma_1\sigma_2$ factor so it will vanish in the σ summation. Let us therefore consider the next to middle terms, which provide the factor $X_1{}^{2m+2}X_2{}^{2m} + X_1{}^{2m}X_2{}^{2m+2}$. These terms vanish when $K \leqslant 2m + 2$.

(b) N, M odd, $L = 1$ or $K = 1$. Let us take $L = 1$, and consider the coefficient of $T_{12}{}^N$. The group of terms with a factor $X_3{}^{3M}$ vanishes in the σ summation, so consider instead those terms with the highest even power $X_3{}^{3(M-1)}$, given by

$$\sum_\sigma X_3{}^{3(M-1)}(\sigma_1 X_1 - \sigma_2 X_2)^{M-1} \times (X_1{}^3 X_2 - X_1 X_2{}^3)(T_1{}^3 T_2 - T_1 T_2{}^3)^N . \tag{A4}$$

(b1) If $M = 4m + 1$ the middle term in the expansion of the $M - 1$ power contributes a term proportional to $-(X_1 X_2)^{2m}$, and when this is combined with other terms we find that they do not vanish unless $K \leqslant 2m + 3$, which is our result in the present case. Note that for $m = 0$ and 1 this condition is trivial.

(b2) If $M = 4m + 3$, the middle term vanishes by the σ summation so we consider instead the next to middle pair $(X_1{}^{2m+2}X_2{}^{2m} + X_1{}^{2m}X_2{}^{2m+2})$. When this is combined with others it implies that we must have $K \leqslant 2m + 5$. For $m = 0$ and 1 this condition is again trivial.

(c) $M = K = 2$, or $N = L = 2$. Take $N = L = 2$. In this case we can choose from the T terms those with one factor of T_2 and T_3, and for X maximum odd power of X_3. The group of terms characterized this way is

$$-\sum_\sigma X_3{}^{3(M-1)}(\sigma_1 X_1 - \sigma_2 X_2)^{M-1} \times (X_1{}^3 X_2 - X_1 X_2{}^3) T_1{}^6 \sigma_1 T_2 T_3 . \tag{A5}$$

Next we take the monomial with maximum odd power in X_2, it is given by $-\Sigma_\sigma X_3{}^{3(M-1)}\sigma_1 X_1 X_2{}^{M-2}(-X_1 X_2{}^3) \times T_1{}^6 \sigma_1 T_2 T_3$. This can vanish only if the rewrite rule is applied to index 1, and then we can read off the rather strong condition $K \leqslant 2$.

(d) M, N odd, $K, L > 1$. Now we take the group of terms with maximum power of X_3 and one power of T_3. They are given by

$$\sum_\sigma X_3{}^{3M}(\sigma_1 X_1 - \sigma_2 X_2)^M (T_1{}^3 T_2 - T_1 T_2{}^3)^{N-1} \times T_3(\sigma_1 T_1{}^3 - \sigma_2 T_2{}^3) . \tag{A6}$$

The two middle terms in the M power survive when combined with suitable T_i terms and the conditions in (b) can be improved:

(d1) $M = 4m + 1$, $K \leqslant 2m + 1$,

(d2) $M = 4m + 3$, $K \leqslant 2m + 2$.

APPENDIX B: MONOMIALS IN THREE VARIABLES

We will now derive the conditions for three-dimensional monomials. Using previous notation we must find out when $S[X^M T^N Y^P, 3]$

$$= \sum_\sigma [X_{12} + X_{23} + X_{31}]^M [T_{12} + T_{23} + T_{31}]^N \times [Y_{12} + Y_{23} + Y_{31}]^P \tag{B1}$$

vanishes under the rewrite rule $X^K T^L Y^Q \to 0$. Here $M + N + P$ is even, $K, L, Q > 0$, and X_{ij}, etc., defined as in (A1). Let us consider the "cyclic" terms with different pairs of indices, say

$$\sum_\sigma X_{12}{}^M T_{23}{}^N Y_{31}{}^P . \tag{B2}$$

When this is expanded it consists of monomials from which no factors can be extracted containing at least $X_i T_i Y_i$ for some i. Thus it cannot vanish due to a rewrite rule, but only due to the σ summation. The σ_i's can be extracted from (B2) and the sum produces a factor

$$\sum_\sigma \sigma_1{}^{M+P}\sigma_2{}^{M+N}\sigma_3{}^{N+P} = (1 + (-1)^M)(1 + (-1)^N)(1 + (-1)^P) , \tag{B3}$$

from which we conclude that the numbers M, N, and P cannot all be even. In the following assume N and M are odd.

Let us next consider

$$\sum_\sigma X_{12}{}^M T_{12} T_{23}{}^{N-1} Y_{31}{}^P . \tag{B4}$$

Here each σ appears with even power so the summation can be ignored, and thus (B4) vanishes only after the rewrite rule. Since only index 1 appears in all three variables, and T_{12} contains T_1 as a single power, we conclude that $L = 1$, and analogously with a specific X_{23} factor that $K = 1$. To get a condition for Q we consider $X_{12}{}^M Y_{12} T_{23}{}^N Y_{23} Y_{31}{}^{P-2}$. It can only vanish when a rewrite rule in index 2 is applied and since Y_2 appears in one term of the product $Y_{12}Y_{23}$ with power 2 we conclude that $Q \leqslant 2$. If $P = 2$ this condition can be improved by considering $X_{12}{}^M T_{12}{}^N Y_{13} Y_{23}$. The rewrite rule can now be applied to indices 1 and 2, and only to these, but both have terms where Y_1 or Y_2 appear singly, therefore $Q = 1$ in this case.

It turns out that in practice we only need $Q = 1$. In that case the above condition is sufficient as well: In the expan-

sion of (B1) we have either terms of type (B2), which vanish due to symmetry, or terms where some index appears in all variables, which vanish by the rewrite rule.

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Spinor focus wave modes

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New solutions of the homogeneous spinor wave equation are obtained. They are similar to the focus wave mode solutions of Maxwell's equations leading to a Gaussian pulse energy. A weighted superposition of these modes may supply finite energy pulses. The particular case of Bessel weight functions is discussed.

I. FUNDAMENTAL MODES

We use Brittingham's procedure[1] for producing nondispersive, packetlike solutions of the spinor wave equation.

Using cylindrical coordinates r, φ, z, and the representation of the Pauli matrices,

$$\sigma_r = \begin{vmatrix} 0 & e^{-i\varphi} \\ e^{i\varphi} & 0 \end{vmatrix}, \quad \sigma_\varphi = \begin{vmatrix} 0 & -ie^{-i\varphi} \\ ie^{i\varphi} & 0 \end{vmatrix}, \quad \sigma_z = \begin{vmatrix} 1 & 0 \\ 0 & -1 \end{vmatrix}, \quad i = \sqrt{-1}, \tag{1}$$

the spinor equation takes the form

$$\begin{aligned} &(\partial_z + (1/c)\partial_t)\psi_1 + e^{-i\varphi}(\partial_r - (i/r)\partial_\varphi)\psi_2 = 0, \\ &e^{i\varphi}(\partial_r + (i/r)\partial_\varphi)\psi_1 - (\partial_z - (1/c)\partial_t)\psi_2 = 0. \end{aligned} \tag{2}$$

Here $\partial_r, \partial_\varphi, \partial_z$, and ∂_t are the derivatives with respect to r, φ, z, and time, respectively, c is the velocity of light, ψ_1, ψ_2 the two components of the spinor field.

Introducing the variables $\xi = z - ct$, $\bar{\xi} = z + ct$ we get

$$\begin{aligned} &2\,\partial_{\bar{\xi}}\,\psi_1 + e^{-i\varphi}(\partial_r - (i/r)\partial_\varphi)\psi_2 = 0, \\ &e^{i\varphi}(\partial_r + (i/r)\partial_\varphi)\psi_1 - 2\,\partial_\xi\psi_2 = 0. \end{aligned} \tag{2'}$$

It is easy to check that Eqs. (2') have the solutions

$$\begin{aligned} \psi_1 &= (f^{\nu-1}/r^\nu)e^{u+i\nu\varphi}, \\ \psi_2 &= -(\lambda f^\nu/r^{\nu+1})e^{u+i(\nu+1)\varphi}, \end{aligned} \tag{3}$$

with

$$u = -((r^2/f) + \lambda\bar{\xi}), \quad f = \mu + \xi/\lambda, \tag{3'}$$

where λ, μ, ν are arbitrary constants.

To obtain a physical interpretation of these solutions we impose the following conditions on λ, μ, ν:

$$\begin{aligned} &\nu = -n-1, \quad n = m/2, \quad m = -1,0,1,2,..., \\ &\lambda = ik, \quad \mu = a/k, \quad ak > 0, \end{aligned} \tag{4}$$

where a, k are real constants. Thus we get from (3), (3'), and (4),

$$\begin{aligned} \psi_1 &= \frac{r^{n+1}}{(a-i\xi)^{n+2}} \exp\left(-\frac{kr^2}{a-i\xi}\right) \\ &\quad \times \exp[-i(k\bar{\xi} + (n+1)\varphi)], \\ \psi_2 &= \frac{-ir^n}{(a-i\xi)^{n+1}} \exp\left(-\frac{kr^2}{a-i\xi}\right) \\ &\quad \times \exp[-i(k\bar{\xi} + n\varphi)]. \end{aligned} \tag{5}$$

This gives three-dimensional nondispersive packetlike solutions propagating at light velocity along 0z. Three dimensional means that amplitude falls off in any direction from the moving pulse center both longitudinally and transversally. Nondispersive means that the pulse envelope shapes remain unchanged along propagation. We conjecture that such solutions of linear partial differential equations exist only in three-dimensional spaces.

Now according to (1) and (5), the components of the current density vector are

$$\begin{aligned} j_r &= e^{i\varphi}\psi_1\psi_2^* + e^{-i\varphi}\psi_1^*\psi_2 \\ &= -\frac{2r^{n+1}\xi}{(a^2+\xi^2)^{n+2}} \exp\left(-\frac{2akr^2}{a^2+\xi^2}\right), \\ j_\varphi &= ie^{i\varphi}\psi_1\psi_2^* - ie^{-i\varphi}\psi_1^*\psi_2 \\ &= -\frac{2r^{n+1}a}{(a^2+\xi^2)^{n+2}} \exp\left(-\frac{2akr^2}{a^2+\xi^2}\right), \\ j_z &= |\psi_1|^2 - |\psi_2|^2 \\ &= \frac{r^{2n}(r^2-\xi^2-a^2)}{(a^2+\xi^2)^{n+2}} \exp\left(-\frac{2akr^2}{a^2+\xi^2}\right), \end{aligned} \tag{6}$$

where the asterisk denotes the complex conjugation. The energy density W is

$$W = |\psi_1|^2 + |\psi_2|^2 = \frac{r^{2n}(r^2+\xi^2+a^2)}{(a^2+\xi^2)^{n+2}} \times \exp\left(-\frac{2akr^2}{a^2+\xi^2}\right), \tag{7}$$

W represents a modulated Gaussian energy pulse. Then the total energy E in a packetlike solution is

$$E = 2\pi \int_0^\infty \int_{-\infty}^{+\infty} Wr\,dr\,d\xi. \tag{8}$$

It is easy to check that E is infinite. To cure this trouble one may think of a cutoff at the lower and upper bounds of the integration in (8). This means that the spinor field is identically zero except when $\xi_1 < \xi < \xi_2$, where the solution (5) is still valid. But this new solution must satisfy the boundary conditions across the surfaces of discontinuities propagating at light velocity along the z axis. These conditions were previously formulated[2] as

$$(\sigma^j\partial_j F + (1/c)\partial_t F)\Psi = 0, \tag{9}$$

where $F = 0$ defines the surface of discontinuity. One sees easily that (5) cannot satisfy (9). Wu and King[3] reached

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similar conclusions for Maxwell's equations (for a more general result see Ref. 4).

II. MODES WITH FINITE ENERGY

As already noticed by Ziolkowski,[5] it is not a drawback *per se* that the solutions (5) have infinite energy. Plane wave solutions also share this property. Nevertheless to appease some critics we show how to construct finite energy solutions.

We first write the solutions (5) in the form

$$\Psi_n = u^n \frac{e^{-kp}}{a-i\xi}\begin{pmatrix} iu \\ 1 \end{pmatrix}, \tag{10}$$

with

$$u = re^{-i\varphi}/(a-i\xi), \quad p = i\bar{\xi} + r^2/(a-i\xi), \tag{10'}$$

and according to Ziolkowski's suggestion,[5] we introduce the Laplace-like transform

$$G(p) = \int_0^\infty F(k)e^{-kp}\,dk, \tag{11}$$

where $F(k)$ is a suitable weight function.

Then we get the new solutions

$$\Phi_n = \frac{u^n}{a-i\xi} G(p)\begin{pmatrix} iu \\ 1 \end{pmatrix} \tag{12}$$

and we have to look for the conditions that $F(k)$ must satisfy to obtain finite energy solutions.

Remark: The inverse transform is

$$F(k) = \int_{-\infty}^{+\infty} d\bar{\xi} \int_{-\infty}^{+\infty} d\xi \int_0^r r\,dr\,K(k,p)G(p) \tag{13}$$

with

$$K(k,p) = [\pi^{-3/2}/(a^2+\xi^2)]\exp[-(\xi/2ka)^2]e^{-kp^*}. \tag{13'}$$

This results from the following relation, which is easy to prove:

$$\int_{-\infty}^{+\infty} d\xi \int_0^\infty r\,dr \int_{-\infty}^{+\infty} d\bar{\xi}\, e^{-k'p}K(k,p) = \delta(k-k'), \tag{14}$$

where $\delta(k-k')$ is the Dirac distribution. If $\Phi_n^\dagger$ denotes the Hermitian conjugate spinor, the energy density W_n for the modes (12) is

$$\begin{aligned} W_n &= \Phi_n^\dagger \Phi_n \\ &= (uu^*)^n(1+uu^*)G(p)G^*(p) \\ &= [r^{2n}(a^2+\xi^2+r^2)/(a^2+\xi^2)^{n+1}]G(p)G^*(p). \end{aligned} \tag{15a}$$

Using the last result together with (11) the total energy E_n,

$$E_n = \int_{-\infty}^{+\infty} d\xi \int_0^\infty r\,dr \int_0^{2\pi} \Phi_n^\dagger \Phi_n\, d\varphi,$$

becomes, after integration on φ,

$$\begin{aligned} E_n = 2\pi &\int_{-\infty}^{+\infty} \frac{d\xi}{(a^2+\xi^2)^{n+2}} \int_0^\infty r^{2n+1}(a^2+\xi^2+r^2)dr \\ &\times \int_0^\infty \int_0^\infty F(k)F^*(k') \\ &\times \exp[-(kp+k'p^*)]dk\,dk' \end{aligned}$$

and changing the order of integrations

$$\begin{aligned} E_n = 2\pi &\int_0^\infty \int_0^\infty dk\,dk'\,F(k)F^*(k') \\ &\times \exp[i(k'-k)\bar{\xi}] \int_{-\infty}^{+\infty} \frac{d\xi}{(a^2+\xi^2)^{n+2}} \\ &\times \int_0^\infty r^{2n+1}(a^2+\xi^2+r^2) \\ &\times \exp\left[-r^2\left(\frac{k}{a-i\xi}+\frac{k'}{a+i\xi}\right)\right] dr. \end{aligned} \tag{15b}$$

From now on, we assume that n is positive integer or half-integer (that is, we discard the solutions with $n=-\frac{1}{2}$ and $n=0$). Then the last integral in the right-hand side of (15b), using the variable $u=r^2$, may be expressed in terms of gamma functions:

$$\begin{aligned} A_n(\xi) &\equiv \frac{1}{2(a^2+\xi^2)^{n+2}} \int_0^\infty u^n(a^2+\xi^2+u^2) \\ &\quad \times \exp\left[-u\left(\frac{k}{a-i\xi}+\frac{k'}{a+i\xi}\right)\right] du \\ &= \frac{1}{2}\left(\frac{\Gamma(n+1)}{(a(k+k')+i\xi(k-k'))^{n+1}}\right. \\ &\quad \left. + \frac{\Gamma(n+2)}{(a(k+k')+i\xi(k-k'))^{n+2}}\right). \end{aligned} \tag{16}$$

Substituting this last result into (15b) gives

$$\begin{aligned} E_n = \pi &\int_0^\infty \int_0^\infty dk\,dk' \exp[i(k-k')\bar{\xi}]F(k)F^*(k') \\ &\times \int_{-\infty}^{+\infty} d\xi\, A_n(\xi). \end{aligned} \tag{17}$$

In the Appendix we prove that for $m>1$ integer or half-integer, x,y real, one has

$$\int_{-\infty}^{+\infty} \frac{dx}{(1+ixy)^m} = f_m \pi\delta(x),$$

$$f_m = \begin{cases} 2/(m-1), & m \text{ integer}, \\ 4/(m-1), & m \text{ half-integer}, \end{cases} \tag{18}$$

where $\delta(x)$ is the Dirac distribution. Since n is positive this gives

$$\begin{aligned} &\int_{-\infty}^{+\infty} \frac{\Gamma(n+1)d\xi}{(a(k+k')+i\xi(k-k'))^{n+1}} \\ &= \frac{\pi f_{n+1}\Gamma(n+1)}{(2ak)^{n+1}} \delta\left(\frac{k-k'}{a(k+k')}\right) \\ &= \frac{\pi f_{n+1}\Gamma(n+1)}{(2ak)^n} \delta(k-k') \end{aligned}$$

using this last result together with (16) and (17), we get

$$\begin{aligned} E_n = &\frac{\pi^2}{(2a)^n} f_{n+1}\Gamma(n+1) \\ &\times \int_0^\infty \frac{dk}{k^n} F(k)F^*(k)\left(1+\frac{n}{2ak}\right), \end{aligned} \tag{19a}$$

so the energy E_n is finite if the integrals T_m,

$$T_m = \int_0^\infty \frac{dk}{k^m} |F(k)|^2, \tag{19b}$$

are bounded for $m = n$ and $m = n + 1$. To satisfy (18) we must assume $n > 1$, which discards the possibilities $n = \frac{1}{2}$, $n = 1$.

III. MODES WITH FINITE ENERGY AND BESSEL WEIGHT FUNCTIONS

We illustrate the previous theory by choosing Bessel weight functions

$$F_{\mu\nu}(kb) = J_\nu(kb) k^{\mu - 1}, \tag{20}$$

where J_ν is the Bessel function of the first kind and νth order, b is a positive scalar, and μ,ν are positive real numbers (μ may be zero).

Then the relation (11) becomes

$$G_{\mu\nu}\left(\frac{p}{b}\right) = \int_0^\infty e^{-pk} J_\nu(kb) k^{\mu - 1}\, dk. \tag{21}$$

This integral exists for $\mu + \nu > 0$ and $\mathrm{Re}(p + ib) > 0$. Both conditions are fulfilled according to the previous requirements. Then[6]

$$G_{\mu\nu}\left(\frac{p}{b}\right) = \frac{(b/2)^\nu}{p^{\mu+\nu}} \left(1 + \frac{b^2}{p^2}\right)^{1/2 - \mu} \frac{\Gamma(\mu + \nu)}{\Gamma(\nu + 1)} \times {}_2F_1\left(\frac{\nu - \mu + 1}{2}, \frac{\nu - \mu}{2} + 1, \nu + 1; -\frac{b^2}{p^2}\right), \tag{22}$$

where ${}_2F_1$ is the hypergeometric function.

Now we have to check the boundedness of the integrals (19b) which become

$$T_{m,\mu\nu} = \int_0^\infty \frac{dk}{k^{m+2-2\mu}} J_\nu^2(kb). \tag{23}$$

They exist for $2\nu + 1 > m + 2 - 2\mu > 0$. Since one has $m = n, n + 1, n > 1$ this leads to the conditions

$$\mu < n/2 + 1 < \nu + \mu, \quad n > 1. \tag{23'}$$

Substituting (21) into (12) gives the solutions $\Phi_{n,\mu\nu}$, which depend on two arbitrary positive lengths a,b and three numbers $n > 1$ integer or half-integer. Then $\mu \geqslant 0$, $\nu > 0$ are compelled to satisfy the two inequalities (23').

The energy density (15a) becomes

$$W_{n,\mu\nu} = \frac{r^{2n}(a^2 + \xi^2 + r^2)}{(a^2 + \xi^2)^{n+1}} \left| G_{\mu\nu}\left(\frac{p}{b}\right)\right|^2. \tag{24}$$

To obtain a clear picture of the energy pulse (24) is not so easy as for the Gaussian mode (7). We shall only discuss its form for $t = 0$ or $z = 0$ and for the set of the lowest integer numbers n,μ,ν, satisfying (23'). To simplify we also assume $a = b$.

For $\mu = 0$ and $\mu = 1$, (22) becomes a very simple expression[6]:

$$G_{0,\nu}\left(\frac{p}{a}\right) = \frac{a^\nu}{\nu} \frac{1}{(p + \sqrt{p^2 + a^2})^\nu}, \tag{25a}$$

$$G_{1,\nu}\left(\frac{p}{a}\right) = \frac{a^\nu}{\sqrt{p^2 + a^2}} \frac{1}{(p + \sqrt{p^2 + a^2})^\nu}, \tag{25b}$$

so for $n = 2$, $\mu = 0$, $\nu = 3$ and $n = 2$, $\mu = 1$, $\nu = 2$ we get from (24), (25a), and (25b)

$$W_{2,03} = \frac{1}{9a^6} \frac{r^4(a^2 + \xi^2 + r^2)}{(a^2 + \xi^2)^3} |\sqrt{p^2 + a^2} - p|^6, \tag{26a}$$

$$W_{2,12} = \frac{1}{a^4} \frac{r^4(a^2 + \xi^2 + r^2)}{(a^2 + \xi^2)^3} \frac{|\sqrt{p^2 + a^2} - p|^4}{|p^2 + a^2|}. \tag{26b}$$

If $|p|^2 \gg a^2$ the last expressions become

$$W_{2,03} = \frac{r^4}{576} \frac{a^2 + \xi^2 + r^2}{(a^2 + \xi^2)^3} \frac{a^6}{|p|^6} \left(1 + O\left(\frac{a^4}{p^4}\right)\right), \tag{27a}$$

$$W_{2,12} = \frac{r^4}{16a^2} \frac{a^2 + \xi^2 + r^2}{(a^2 + \xi^2)^3} \times \frac{a^6}{|p|^6} \left|1 - \frac{a^2}{p^2}\right| \left(1 + O\left(\frac{a^4}{p^4}\right)\right), \tag{27b}$$

where O is the Bachmann–Landau symbol for the order of a quantity. For $|p|^2 \ll a^2$, we get

$$W_{2,03} = \frac{r^4}{9} \frac{a^2 + \xi^2 + r^2}{(a^2 + \xi^2)^3} \left|1 - \frac{p}{a}\right|^6 \left(1 + O\left(\frac{p^2}{a^2}\right)\right), \tag{28a}$$

$$W_{2,12} = \frac{r^4}{a^2} \frac{a^2 + \xi^2 + r^2}{(a^2 + \xi^2)^3} \left|1 - \frac{p}{a}\right|^4 \left(1 + O\left(\frac{p^2}{a^2}\right)\right). \tag{28b}$$

Now according to (10') one has

$$|p|^2 - a^2 = \frac{(r^2 + z^2 - c^2t^2 - a^2)(r^2 + z^2 - c^2t^2 + a^2) + 4a^2zct}{a^2 + \xi^2}, \tag{29}$$

which simplifies for $t = 0$ and $z = 0$.

At $t = 0$ the condition $|p|^2 \gg a^2$ is fulfilled for $R^2 \equiv r^2 + z^2 \gg a^2$ and one has

$$|p|^2 = [R^4/(a^2 + z^2)](1 + O(a^2/R^2)). \tag{30}$$

Substituting (30) into (27) gives

$$W_{2,03} = \frac{a^6 r^4}{576 R^{10}} \left(1 + O\left(\frac{a^2}{R^2}, \frac{a^4}{p^4}\right)\right), \tag{31a}$$

$$W_{2,12} = \frac{a^4 r^4}{16 R^{10}} \left(1 + O\left(\frac{a^2}{R^2}, \frac{a^4}{p^4}\right)\right), \tag{31b}$$

when $R \to \infty$ these expressions decrease to zero as R^{-10}. Now for $R^2 \ll a^2$ one has

$$\left|1 - \frac{p}{a}\right|^2 = 1 + O\left(\frac{r^2}{a^2}, \frac{z^2}{a^2}\right) \tag{32}$$

and from (28) we get

$$W_{2,03} = \frac{r^4}{9a^4} \left(1 + O\left(\frac{r^2}{a^2}, \frac{z^2}{a^2}, \frac{p^2}{a^2}\right)\right), \tag{33a}$$

$$W_{2,12} = \frac{r^4}{a^6} \left(1 + O\left(\frac{r^2}{a^2}, \frac{z^2}{a^2}, \frac{p^2}{a^2}\right)\right). \tag{33b}$$

For $r \mapsto 0$ these expressions decrease to zero as r^4.

Let us now consider what happens on the sphere $R^2 = a^2$ which corresponds to $|p|^2 = a^2$. There, of course, one must consider the exact expressions (26). Still using (10') with the condition $R^2 = a^2$ a simple calculation gives

$$|\sqrt{p^2+a^2} - p|^2 = a^2 + a(p+p^*) - a\sqrt{p+p^*}(\sqrt{p}+\sqrt{p^*}), \tag{34}$$

with

$$\begin{aligned} p + p^* &= 2ar^2/(a^2+z^2), \\ \sqrt{p}+\sqrt{p^*} &= 2a^{3/2}/\sqrt{a^2+z^2}. \end{aligned} \tag{34'}$$

Substituting (34') into (34) gives

$$|\sqrt{p^2+a^2} - p|^2 = [a^2/(a^2+z^2)](a\sqrt{2}-r)^2. \tag{35}$$

From (24) and (35) we get

$$W_{2,03} = [2a^2r^4/9(a^2+z^2)^6](a\sqrt{2}-r)^6, \tag{36a}$$

$$W_{2,12} = [r^4/(a^2+z^2)^4](a\sqrt{2}-r)^4. \tag{36b}$$

These results show that the energy density decreases swiftly to zero far from the sphere $R^2 = a^2$ where it is bounded.

For $z = 0$ one obtains similar conclusions: $W_{2,03} = W_{1,2} \Rightarrow 0$ when $|p|^2 \gg a^2$ outside the hyperboloid H_1; $r^2 - c^2t^2 - a^2 = 0$, and when $|p|^2 \ll a^2$ inside the hyperboloid H_2; $r^2 - c^2t^2 + a^2 = 0$, the energy density being non-null and bounded on both hyperboloids.

Although limited to $t = 0$ and $z = 0$, the picture of the energy pulse makes clear that it is focused around some hypersurface. At least for $\mu = 0$ and $\mu = 1$, it is also clear from (25a) and (25b), that for n fixed, higher values of ν increase the energy concentration.

IV. CONCLUSION

The Laplace-like transform of the fundamental modes (5) gives a rich class of possible solutions of the spinor wave equation since the weight function $F(k)$ is somewhat arbitrary. In fact the condition that the integrals T_m are bounded is rather mild. We only investigated the case of Bessel weight functions and we found a quintuple infinity of solutions depending on two real scalars and three positive numbers.

Of course many questions are still unanswered. Are these solutions only a mathematical curiosity or do they have a physical support? In this last case what is the role and the meaning of the weight function? Clearly further investigation is needed to master these issues.

APPENDIX: PROOF OF EQ. (18)

We prove here the relation

$$F_m(x) = \int_{-\infty}^{+\infty} \frac{dy}{(1+ixy)^m} = f_m \pi \delta(z), \quad i = \sqrt{-2}, \tag{A1}$$

for $m \geqslant 1$ integer or half-integer and x,y real, $\delta(x)$ is the Dirac distribution, and f_m a constant depending upon m.

We first introduce the functions $F_{m,\alpha}(x)$ with $\alpha > 0$:

$$F_{m,\alpha}(x) = \int_{-\alpha}^{\alpha} \frac{dy}{(1+ixy)^m}. \tag{A2}$$

Then if φ is a function with bounded support, we get

$$\langle F_m, \varphi \rangle = \lim_{\alpha \to \infty} \int_a^b F_{m,\alpha}(x)\varphi(x)dx \tag{A3}$$

for any interval (a,b) containing the support of φ. Let $G_{m,\alpha}(x)$ be the functions

$$G_{m,\alpha}(x) = \int_{-\infty}^{x} F_{m,\alpha}(x)dx. \tag{A4}$$

Integrating (A3) by parts and using $\varphi(a) = \varphi(b) = 0$ gives

$$\langle F_m, \varphi \rangle = -\lim_{\alpha \to \infty} \int_a^b \varphi'(x) G_{m,\alpha}(x)dx, \tag{A5}$$

we now assume that the two following conditions are fulfilled.

(i) $G_{m,\alpha}(x)$ converges in mean to the Heavside function $H(x)$:

$$\lim_{(\alpha \to \infty)} G_{m,\alpha}(x) = f_m \pi H(x), \tag{A6}$$

that is,

$$\lim_{\alpha \to \infty} \int_a^b G_{m,\alpha}(x)dx = f_m \pi b \tag{A7}$$

with zero inside (a,b).

(ii) For $x > 0$, $G_{m,\alpha}(x)$ is bounded by $f_m \pi$:

$$G_{m,\alpha}(x) \leqslant f_m \pi. \tag{A8}$$

The two conditions imply

$$\lim_{\alpha \to \infty} \int_a^b \varphi'(x) G_{m,\alpha}(x)dx = f_m \pi \int_a^b \varphi'(x)H(x)dx, \tag{A9}$$

and substituting (A9) into (A5) gives $\langle F_m, \varphi \rangle = f_m \pi \varphi(0)$, which is (A1).

Now to prove (A9) we start[7] with

$$\left| \lim_{\alpha \to \infty} \int_a^b (G_{m,\alpha}(x) - f_m \pi H(x))\varphi'(x)dx \right|$$

$$\leqslant \operatorname*{lub}_{a<x<b} |\varphi'(2)| \int_a^b |G_{m,\alpha}(x) - f_m \pi H(2)|dx,$$

but using (A6) and (A7) one has

$$\lim_{\alpha \to \infty} \int_a^b |G_{m,\alpha}(x) - f_m \pi H(x)|dx$$

$$= \lim_{\alpha \to \infty} \int_a^b (G_{m,\alpha}(x) - f_m \pi H(x))dx = 0,$$

which leads to (A9).

Let us now discuss the condition (A6) starting with $m > 1$ integer. From (A2) we get

$$F_{m,\alpha}(x) = \frac{-1}{ix(m-1)} \times \left(\frac{1}{(1+i\alpha x)^{m-1}} - \frac{1}{(1-i\alpha x)^{m-1}} \right) \tag{A10}$$

and using (A4)

$$G_{m,\alpha}(x) = \frac{-1}{i(m-1)} \int_{-\infty}^{x} \left(\frac{1}{(1-i\alpha x)^{m-1}} - \frac{1}{(1-i\alpha x)^{m-1}} \right) \frac{dx}{x}, \tag{A11}$$

but one has

$$\int \frac{dx}{x(ax+b)^m} = \frac{-1}{mb}\left(\log\left(\frac{ax+b}{x}\right) - \sum_{k=1}^{m-1}\binom{m-1}{k}\frac{(-a)^k x^k}{k(ax+b)^k}\right),$$

so (A11) may be written

$$G_{m,\alpha}(x) = G^0_{m,\alpha}(x) + g_{m,\alpha}(x), \tag{A12}$$

with

$$G^0_{m,\alpha}(x) = [2/(m-1)](\arctan \alpha x + \pi/2), \tag{A13}$$

$$g_{m,\alpha}(x) = \frac{-1}{i(m-1)}\sum_{k=1}^{m-2}\binom{m-2}{k}\frac{x^k}{k} \times\left(\frac{(1-i\alpha)^k}{(1+i\alpha x)^k} - \frac{(1+i\alpha)^k}{(1-i\alpha x)^k}\right), \tag{A14}$$

where we used the fact that $g_{m,\alpha}(x)\mapsto 0$ for $x\mapsto -\infty$ as easily seen by writing the term into brackets

$$[1/(1+\alpha^2x^2)^k]\,[(1/x - i\alpha - i\alpha x - \alpha^2x^2)^k - (1/x + i\alpha + i\alpha x - \alpha^2x^2)^k].$$

Using the relation

$$\int \arctan \alpha x\, dx = x \arctan \alpha x - (1/2\alpha)\log(1+\alpha^2x^2), \tag{A15}$$

we get

$$\int_a^b G^0_{m,\alpha}(x)dx = \frac{2}{m-1}\left((b-a)\frac{\pi}{2} + b\arctan \alpha b - a\arctan \alpha a - \frac{1}{2\alpha}\log\left(\frac{1+\alpha^2b^2}{1+\alpha^2a^2}\right)\right)$$

which gives, if zero is inside (a,b),

$$\lim_{\alpha\mapsto\infty}\int_a^b G^0_{m,\alpha}(x)dx = \frac{2\pi b}{m-1}. \tag{A16}$$

Let us now consider (A14). One has

$$\int_a^b g_{m,\alpha}(x)dx = \frac{-1}{i(m-1)}\sum_{k=1}^{m-2}\frac{1}{k}\binom{m-2}{k} \times\int_a^b\left(\frac{(1-i\alpha)^kx^k}{(1+i\alpha x)^k} - \frac{(1+i\alpha)^kx^k}{(1-i\alpha x)^k}\right)dx,$$

but according to the mean theorem there exist x_1, x_2 in (a,b) such that

$$\int_a^b\left(\frac{(1-i\alpha)^kx^k}{(1+i\alpha x)^k} - \frac{(1+i\alpha)^kx^k}{(1-i\alpha x)^k}\right)dx = \frac{(1-i\alpha)^kx_1^k}{(1+i\alpha x_1)^k} - \frac{(1+i\alpha)^kx_2^k}{(1-i\alpha x_2)^k},$$

which is zero for $\alpha\mapsto\infty$ so that

$$\lim_{\alpha\mapsto\infty}\int_a^b g_{m,\alpha}(x)dx = 0. \tag{A17}$$

Finally, from (A12), (A16), and (A17) we get

$$\lim_{\alpha\mapsto\infty}\int_a^b G_{m,\alpha}(x)dx = \frac{2\pi b}{m-1}, \tag{A18}$$

which is (A7) with $f_m = 2/(m-1)$.

To prove the condition (A8), we just have to remark that according to (A11), $G_{m,\alpha}(x)$ is a decreasing function of m, so one has

$$G_{m,\alpha}(x) \leqslant \frac{-1}{i(m-1)}\int_{-\infty}^{x}\left(\frac{1}{1+i\alpha x} - \frac{1}{1-i\alpha x}\right)dx = \frac{2}{m-1}\left(\arctan \alpha x + \frac{\pi}{2}\right) \leqslant \frac{2\pi}{m-1}$$

in agreement with (A8).

We now consider the case m half-integer, with $p\geqslant 1$ one has

$$F_{(2p+1)/2,\alpha}(x) = \frac{-2}{i(2p-1)x} \times\left(\frac{1}{(1+i\alpha x)^{(2p-1)/2}} - \frac{1}{(1-i\alpha x)^{(2p-1)/2}}\right)$$

and

$$G_{(2p+1)/2,\alpha}(x) = \frac{-2}{i(2p-1)}\left(\int_{-\infty}^{x}\frac{dx}{x(1+i\alpha x)^{(2p-1)/2}} - \int_{-\infty}^{x}\frac{dx}{x(1-i\alpha x)^{(2p-1)/2}}\right). \tag{A19}$$

Using the relation

$$\int_{-\infty}^{x}\frac{dx}{x(1\pm i\alpha x)^{(2p-1)/2}} = \frac{2}{(2p-3)(1\pm i\alpha x)^{(2p-3)/2}} + \int_{-\infty}^{x}\frac{dx}{x(1\pm i\alpha x)^{(2p-3)/2}}.$$

We may write (A19) for $p\geqslant 2$:

$$G_{(2p+1)/2,\alpha}(x) = [(2p-3)/(2p-1)]G_{(2p-1)/2,\alpha}(x) + g_{(2p+1)/2,\alpha}(x), \tag{A20}$$

with

$$g_{(2p+1)/2,\alpha}(x) = \frac{-4}{i(2p-1)(2p-3)} \times\left(\frac{1}{(1+i\alpha x)^{(2p-3)/2}} - \frac{1}{(1-i\alpha x)^{(2p-3)/2}}\right). \tag{A21}$$

But one has

$$\lim_{\alpha\mapsto\infty}\int_a^b g_{(2p+1)/2,\alpha}(x)dx = 0,$$

so it becomes, for $p\geqslant 2$,

$$\lim_{\alpha\mapsto\infty}\int_a^b G_{(2p+1)/2,\alpha}(x)dx = \frac{2p-3}{2p-1}\lim_{\alpha\mapsto\infty}\int_a^b G_{(2p-1)/2}(x)dx. \tag{A22}$$

Now for $p=1$, one has

$$F_{3/2,\alpha}(x) = \frac{-2}{ix}\left(\frac{1}{(1+i\alpha x)^{1/2}} - \frac{1}{(1-i\alpha x)^{1/2}}\right),$$

$$G_{3/2,\alpha}(x) = 8(\arctan \alpha x + \pi/2)$$

and using (A15) we get

$$\lim_{\alpha \to \infty} \int_a^b G_{3/2,\alpha}(x)dx = 8\pi b. \tag{A23}$$

Substituting (A23) into (A22) gives

$$\lim_{\alpha \to \infty} \int_a^b G_{(2p+1)/2,\alpha}(x)dx = \frac{8\pi b}{2p-1} = \frac{4\pi b}{m-1}, \tag{A24}$$

which is (A7) with $f_m = 4/(m-1)$. The proof (A8) is as for m integer.

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The anharmonic oscillator at a finite temperature. Comparison of quantum and classical stochastic calculations

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An oscillator with a small, but otherwise arbitrary, perturbing potential is considered immersed in a random cavity radiation. Classical (stochastic) calculations are done when the radiation has a Rayleigh–Jeans spectrum and a complete Planck spectrum (i.e., with zero point). These are compared with the results obtained by a quantum calculation. First, a comparison is made of stationary values, in particular, the energy. Then the emission and the absorption spectra are calculated, in particular, the absorption spectrum for an arbitrary incoming radiation. Finally, a detailed comparison is made of the absorption bands when the perturbing potential has the form λx^{2K} $(K = 2,3,...)$. In all cases, it is explicitly shown that the quantum and the classical behavior agree in the limit of high temperatures. It is also shown that the classical system immersed in a radiation with complete Planck spectrum is much closer to the quantum system than the fully classical system (with a Rayleigh–Jeans spectrum).

I. INTRODUCTION

The problem of the equilibrium between radiation and matter was historically at the origin of quantum theory.[1] It is natural, therefore, to return to this problem for a better understanding of the transition from quantum to classical electrodynamics. With this purpose, we shall compare the emission and absorption of radiation by a simple system according to both quantum and classical theories. For the sake of simplicity it is convenient to deal with time-independent problems, and this can be accomplished by considering the system immersed in a cavity radiation at a given temperature. As the temperature increases, quantum and classical behavior approach each other and we may study how this approaching occurs. For instance, we can see how the discrete spectrum characteristic of quantum theory transforms into the continuous classical spectrum.

In particular, we shall study the approaching of the quantum formulas to the classical ones with the decrease of the dimensionless parameter $\hbar\omega_0/k_B T$, where T is the absolute temperature and ω_0 a typical frequency of the system under study. This provides a physical example of the formal limit $\hbar \to 0$. In our case the above dimensionless parameter can be made arbitrarily small by just increasing the temperature (our nonrelativistic treatment has the constraint $\hbar\omega_0 \ll mc^2$, but the classical limit can be obtained well before this restriction is relevant).

As it is well known, cavity radiation has a Rayleigh–Jeans spectrum according to classical theory and a Planck spectrum in quantum theory. It is also possible to consider an intermediate case, namely a classical system immersed in a Planck's cavity radiation. In this case it is more appropriate to take the complete Planck's law, i.e., including a zero point random field, which leads to a theory known as stochastic electrodynamics.[2] This theory, which has received continued attention during the last 30 years, was considered at the beginning as a possible alternative for quantum electrodynamics. Indeed the theory is able to interpret a number of phenomena previously considered as purely quantal, but it has failed in some essential points, like the inability to give even a qualitative explanation of the discrete spectra of atoms. As a result of the work made in the last decade,[2–5] it is now clear that stochastic electrodynamics is just an intermediate theory between quantum and conventional classical electrodynamics and, therefore, it is most appropriate for the study of the classical limit of quantum theory.

An interesting question is whether some modification of stochastic electrodynamics, under the same spirit, could be closer to quantum theory. One of the purposes of the work here reported has been the search for ideas about the direction in which such modification should be made. It seems to us that these ideas might be most likely found in the study of semiclassical situations, such as a system immersed in cavity radiation at a high temperature, which is the study here reported.

The simplest system is the harmonic oscillator, and it has been studied many times according to stochastic electrodynamics, both at zero and at a finite temperature. However, this system gives relatively little information because it interacts with only a narrow band of frequencies. The next simple system is the oscillator perturbed by a small anharmonic potential which can be treated as a perturbation, and this is the system we study.

As a by-product of our calculation, explicit expressions are obtained for several quantities associated with a (stochastic) classical system immersed in an arbitrary random radiation. These formulas could be useful in other areas of mathematical physics.

In Sec. II we calculate the system in equilibrium with cavity radiation both classically and quantum mechanically. In Sec. III we consider in detail the absorption and emission of radiation of the quantum system and in Secs. IV and V the corresponding classical cases. In Sec. VI we compare the quantum and classical emission spectra as the temperature increases for the particular cases of potentials of the form λx^{2K}. Finally, in Sec. VII we discuss the results obtained.

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II. THE SYSTEM IN EQUILIBRIUM WITH RADIATION

We consider an anharmonic oscillator in one dimension as the simplest nontrivial system. We assume an arbitrary potential $\lambda V(x)$, where λ is used as an expansion parameter. The Hamiltonian is, therefore,

$$H = H_0 + \lambda V(x), \quad H_0 = p^2/2m + \tfrac{1}{2}m\omega_0^2 x^2, \tag{2.1}$$

with an obvious meaning for the variables.

As it is well known, the classical cavity (or blackbody) radiation has the Rayleigh–Jeans spectrum and the statistical ensemble of systems in equilibrium with this radiation is the canonical ensemble, having a Maxwell–Boltzmann probability distribution in phase space. All thermodynamic properties of the system can be obtained from the partition function which, for our system, is

$$\begin{aligned} Z_{\rm cl}(\beta) &= \int e^{-\beta H}\, dx\, dp \\ &= \int e^{-\beta H_0}(1-\beta\lambda V)\, dx\, dp + O(\lambda^2) \\ &= (2\pi/\beta\omega_0)(1-\beta\lambda\langle V\rangle_{\rm cl}) + O(\lambda^2), \end{aligned} \tag{2.2}$$

where $\beta \equiv 1/k_B T$ is the inverse of the absolute temperature times Boltzmann's constant and

$$\langle V\rangle_{\rm cl} \equiv \sqrt{\beta m/2\pi}\,\omega_0 \int_{-\infty}^{\infty} V(x)\exp\left(-\frac{1}{2}\beta m\omega_0^2 x^2\right)dx. \tag{2.3}$$

From (2.2) it is easy to obtain the average energy, which is

$$\langle E\rangle_{\rm cl} = -\frac{d}{d\beta}\ln Z_{\rm cl} = \beta^{-1} + \lambda\langle V\rangle_{\rm cl} + \beta\lambda\frac{d}{d\beta}\langle V\rangle_{\rm cl} + O(\lambda^2). \tag{2.4}$$

For the quantum calculation, we shall represent by $|n\rangle$ the eigenvectors of the Hamiltonian operator, H_0, $(n+\frac{1}{2})\hbar\omega_0$ being the corresponding eigenvalues. The eigenvalues and eigenvectors of the complete Hamiltonian, H, will be represented by E_n and $|\phi_n\rangle$, respectively. To first order in λ we have

$$E_n = (n+\tfrac{1}{2})\hbar\omega_0 + \lambda V_n, \quad V_n \equiv \langle n|V|n\rangle. \tag{2.5}$$

The quantum blackbody radiation has a Planck spectrum and the quantum canonical ensemble in equilibrium is represented by the density matrix

$$\hat{\rho} = (\mathrm{Tr}\, e^{-\beta H})^{-1} e^{-\beta H} = Z_Q^{-1}\sum_{n=0}^{\infty} |\phi_n\rangle e^{-\beta E_n}\langle\phi_n|, \tag{2.6}$$

where the partition function is, to order λ,

$$\begin{aligned} Z_Q = \mathrm{Tr}\, e^{-\beta H} &\simeq \mathrm{Tr}[e^{-\beta H_0}(1-\lambda\beta V)] \\ &= \tfrac{1}{2}\,\mathrm{csch}(\tfrac{1}{2}\beta\hbar\omega_0)(1-\beta\lambda\langle V\rangle_Q). \end{aligned} \tag{2.7}$$

The expectation $\langle V\rangle_Q$ can be easily calculated taking into account that the probability density of the position coordinate of a harmonic oscillator at a finite temperature is a Gaussian.[6] It is obtained

$$\langle V\rangle_Q = \left[\left(\frac{m\omega_0}{\pi\hbar}\right)\tanh\left(\frac{1}{2}\beta\hbar\omega_0\right)\right]^{1/2}\int_{-\infty}^{\infty} dx\, V(x) \times \exp\left[-\left(\frac{m\omega_0}{\hbar}\right)\tanh\left(\frac{1}{2}\beta\hbar\omega_0\right)x^2\right]. \tag{2.8}$$

From the partition function, the average energy is easily obtained to be

$$\langle E\rangle_Q = -\frac{d}{d\beta}\ln Z_Q = \frac{1}{2}\hbar\omega_0\tanh\left(\frac{1}{2}\beta\hbar\omega_0\right) + \lambda\langle V\rangle_Q + \beta\lambda\frac{d}{d\beta}\langle V\rangle_Q. \tag{2.9}$$

It can be realized that, in the high temperature limit, $\beta\to 0$, Eq. (2.7) goes to Eq. (2.2), except for the irrelevant multiplicative constant $\hbar/2\pi$, as it should. Then, all thermodynamics quantities agree in this limit, for instance the energy (2.9) tends to (2.4).

Now, we must consider the situation in stochastic electrodynamics. We assume a purely classical ensemble immersed in a complete Planck's blackbody radiation (i.e., including the zero point field). In this case, no full equilibrium is possible because, as it is well known, the unique radiation in equilibrium with a classical system has a Rayleigh–Jeans spectrum.[7] We may consider, however, the stationary ensemble, whose rate of emission is exactly balanced by absorption, although the balance at each frequency no longer holds. In a sense, the system is in equilibrium with the radiation, but the radiation is not stationary (its spectrum is changing). It is necessary to assume, therefore, that the cavity where the system is enclosed is indefinitely large so that the action of the system on the radiation is negligible. In these conditions it is possible to calculate the stationary probability distribution by Markov approximation techniques.[3,4,8] This technique can be summarized as follows.

The starting point is the classical equation of motion of a charged particle under the action of a force derived from the potential (2.1) and immersed in a radiation field. It is

$$m\ddot{x} = -m\omega_0^2 x - \lambda\frac{dV}{dx} - \frac{2e^2}{3mc^3}\dddot{x} + e\mathscr{E}, \tag{2.10}$$

where the third term in the right-hand side represents the damping due to the reaction on the particle by the field emitted by it, and the last term is the force due to the radiation field. We work in the electric dipole approximation, which consists of neglecting the dependence of $\mathscr{E}$ on the coordinate x. The electric field, $\mathscr{E}(t)$, depends only on time and it can be considered a stochastic process, so that Eq. (2.10) is a nonlinear stochastic differential equation with a nonwhite noise. Then, the technique of the Markov approximation consists of solving first the classical dynamical problem [i.e., Eq. (2.10) without the last two terms], so finding the possible orbits (periodic motions) of the system.

The motion along an orbit of energy E can be represented by

$$x(E,t) = \sum_n x_n(E)e^{in\omega(E)t}. \tag{2.11}$$

The frequency as a function of the energy can be calculated by using canonical perturbation methods.[9] It is given to order λ by

$$\omega(E) = \omega_0\left(1 + \frac{\omega_0}{2\pi}\lambda\frac{d}{dE}\oint V\right), \tag{2.12}$$

where

$$\oint V \equiv \int_0^{2\pi/\omega_0} V\left(\sqrt{\frac{2E}{m\omega_0^2}}\cos\omega_0 s\right)ds. \tag{2.13}$$

For later convenience, we give the expression of $|x_1|^2$ as a function of E, to order λ, obtained from the same canonical perturbation techniques,[9]

$$|x_1(E)|^2 = (E/2m\omega_0^2)\times\left[1 - \left(\frac{\lambda\omega_0}{2\pi E}\right)\oint V + \frac{\lambda\omega_0}{2\pi E}\frac{d}{dE}\left(E\oint V_c\right)\right], \tag{2.14}$$

where

$$\oint V_c \equiv \int_0^{2\pi/\omega_0} V\left(\sqrt{\frac{2E}{m\omega_0^2}}\sin\omega_0 s\right)\cos 2\omega_0 s\, ds. \tag{2.15}$$

As concerns the action of the last two terms, it can be considered as a perturbation with a characteristic time large enough for the existence of an intermediate time scale, such that the diffusion of the orbits is approximately Markovian.[4,8] The Markov approximation can be then considered a lowest-order approximation in the coupling between the system and the radiation, i.e., second order in the electric charge e. It is therefore the classical counterpart of the first order approximation in the fine structure constant $\alpha \equiv e^2/\hbar c$ so frequently used in quantum electrodynamics (QED). In our classical system, the relevant small dimensionless parameter is $\gamma \equiv 2e^2\omega_0/3mc^3$.

In the Markov approximation it is possible to calculate the stationary ensemble immersed in an arbitrary but isotropic homogeneous radiation. If we denote by $S_{\mathscr{E}}$ the spectrum of the field, i.e.,

$$S_{\mathscr{E}}(\omega) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\theta\,\langle\mathscr{E}(t+\theta)\mathscr{E}(t)\rangle e^{i\omega\theta}, \tag{2.16}$$

which is related to the radiation energy density per unit volume and unit frequency interval $u(\omega)$, by the relation,

$$S_{\mathscr{E}}(\omega) = (2\pi/3)u(\omega), \tag{2.17}$$

the stationary probability distribution of the ensemble is, to first order in λ,[3,4,6]

$$\rho_{\rm st}(E)dE = C\exp\left[-\int_0^E dE'\,\frac{2\omega^2(E')}{3c^3\pi S_{\mathscr{E}}(\omega(E'))}\right]\frac{2\pi}{\omega(E)}\,dE, \tag{2.18}$$

where $2\pi/\omega(E)$ is the period of an orbit of the oscillator as a function of the energy and C is a normalization constant such that the integral of (2.18) from 0 to ∞ is unity. The period of the orbit appears in (2.18) multiplying dE as a consequence of the transformation from phase space variables $\{x, p\}$ to the energy variable E. It can be realized that, in the case of a Rayleigh–Jeans spectrum, $u(\omega) \propto \omega^2$, and (2.18) leads to (2.2).

The most interesting spectra fulfill the Wien law, which means that β appears only in the combination, $\beta\omega$, i.e.,

$$S_{\mathscr{E}}(\omega) = (2\hbar\omega^3/3\pi c^3)\phi(\beta\hbar\omega). \tag{2.19}$$

Note that $\hbar$ enters here just as a constant of action needed in order to make dimensionless the argument of ϕ, but it is not necessarily associated with quantum theory. As is well known, both Rayleigh–Jeans and Planck's spectra fulfill (2.19) with ϕ given by

$$\phi_{\rm RJ}(\epsilon) = \epsilon^{-1}, \quad \phi_{\rm P}(\epsilon) = (e^{\epsilon}-1)^{-1}, \quad \phi_{\rm PC}(\epsilon) = \tfrac{1}{2} + (e^{\epsilon}-1)^{-1}. \tag{2.20}$$

The function $\phi_{\rm PC}$ corresponds to the complete Planck spectrum, including the zero point field. Substituting (2.19) into (2.18) we get

$$\rho_{\rm st}(E)dE = C\exp\left[-\int_0^E \frac{dE'}{\hbar\omega(E')\phi(\beta\hbar\omega(E'))}\right]\frac{2\pi}{\omega(E)}\,dE. \tag{2.21}$$

It is not possible in general to define a partition function, associated with (2.21) and having the usual properties of allowing us to get all thermodynamic quantities. However, these quantities can be calculated directly from (2.21). For instance, the average energy is[10]

$$\langle E\rangle = \hbar\omega_0\phi(\beta\hbar\omega_0) + (\lambda\hbar^2\beta/2)\phi'(\beta\hbar\omega_0)\langle V''\rangle + \lambda\langle V\rangle, \tag{2.22}$$

where the mean values correspond to the harmonic oscillator, namely, by taking $\omega(E) \equiv \omega_0$ in (2.21). After a little algebra, it is easy to see that this expression agrees with the quantum one (2.9) if we take for ϕ the last expression (2.20), i.e., the Planck spectrum with zero point, which is the one usually associated with stochastic electrodynamics. This fact shows that this theory is indeed intermediate between classical and quantum electrodynamics, and also that the Planck spectrum should include the zero point in this context. Note that the full probability distribution of the energy (2.21) does not agree with the quantum one, as also there is no agreement for $\langle E\rangle$ to second order in λ [3].

III. EMISSION AND ABSORPTION IN QUANTUM ELECTRODYNAMICS

The probability per unit time of spontaneous emission from the state $|\varphi_n\rangle$ to the state $|\varphi_k\rangle$ is given, in quantum electrodynamics, by the Einstein coefficient

$$A_{nk} = (4e^2\omega_{nk}^3/3\hbar c^3)|\langle\varphi_n|\hat{x}|\varphi_k\rangle|^2 \tag{3.1}$$

with

$$\omega_{nk} = (E_n - E_k)/\hbar = (n-k)\omega_0 + (\lambda/\hbar)(V_n - V_k). \tag{3.2}$$

The matrix elements in (3.1) are of order λ for $n - k \neq 1$, and thus only the coefficients $A_{n,n-1}$ are not zero at this order. The quantum mechanical perturbation theory gives for these coefficients, which we shall represent simply by A_n, the expression

$$A_n = \frac{2e^2\omega_0^2}{3mc^3} n\left[1 + \frac{\lambda}{\hbar\omega_0}\left(\frac{(V\hat{a}^2)_n - (V\hat{a}^2)_{n+1}}{n}\right) + \frac{3\lambda}{\hbar\omega_0}(V_n - V_{n-1})\right], \quad n = 1,2,\ldots, \tag{3.3}$$

$\hat{a}$ being the annihilation operator.

The spectrum of the anharmonic oscillator consists, therefore, of a set of lines at the frequencies

$$\omega_n = \omega_0[1 + (\lambda/\hbar\omega_0)(V_n - V_{n-1})], \quad n = 1,2,\ldots. \tag{3.4}$$

Each line has a width equal to $A_n + A_{n-1}$, and the line spectrum becomes a continuous one when the separation between neighbor lines is of the order of half the sum of the two linewidths, i.e.,

$$\frac{2\hbar^2\omega_0^2}{3mc^2}\left(\frac{e^2}{\hbar c}\right) \simeq \frac{\lambda(V_n - 2V_{n-1} + V_{n-2})}{2(n-1)}. \tag{3.5}$$

Now we consider a mixed state of the anharmonic oscillator having density matrix

$$\hat{\rho} = \sum_{n=0}^{\infty} |\varphi_n\rangle p_n \langle\varphi_n|, \quad p_n \geqslant 0. \tag{3.6}$$

The energy spontaneously emitted per unit time and unit frequency interval is (neglecting linewidths),

$$I_e^Q(\omega) = \sum_n I_{e,n}^Q \delta(\omega - \omega_n) + O(\lambda^2), \tag{3.7}$$

where

$$I_{e,n}^Q = p_n \hbar\omega_n A_n. \tag{3.8}$$

We are interested in the ensemble in equilibrium with blackbody radiation, i.e., the canonical ensemble such that

$$\hat{\rho} = \frac{e^{-\beta\hat{H}}}{\mathrm{Tr}(e^{-\beta\hat{H}})} \Leftrightarrow p_n = \frac{e^{-\beta E_n}}{\Sigma_n e^{-\beta E_n}}. \tag{3.9}$$

After a lengthy but straightforward calculation it is obtained for the total emitted power

$$W_e^Q \equiv \sum_n I_{e,n}^Q = \frac{2e^2\hbar\omega_0^3}{3mc^3}\phi_P(\beta\hbar\omega_0)\left[1 + \frac{\lambda}{2m\omega_0^2}\left(3 + \beta\hbar\omega_0\frac{\phi_P'(\beta\hbar\omega_0)}{\phi_P(\beta\hbar\omega_0)}\right)\langle V''\rangle_Q\right], \tag{3.10}$$

where $\phi_P(\epsilon)$ is given by Planck's formula (2.20), and [compare with (2.8)]

$$\langle V''\rangle_Q = \mathrm{Tr}\left(\hat{\rho}\frac{d^2V}{dx^2}\right) = \left[\frac{m\omega_0}{\pi\hbar}\tanh\left(\frac{1}{2}\beta\hbar\omega_0\right)\right]^{1/2}\int_{-\infty}^{\infty} dx\, V''(x) \times \exp\left[-\frac{m\omega_0}{\hbar}\tanh\left(\frac{1}{2}\beta\hbar\omega_0\right)x^2\right]. \tag{3.11}$$

The next step is the calculation of the absorption and the stimulated emission when the system is immersed in an electromagnetic field with energy density per unit frequency, $u(\omega)$. The two processes cannot be separated physically and we shall calculate both simultaneously. The net energy absorbed by the system per unit time and unit frequency interval, in the state given by (3.9), is

$$I_a^Q(\omega) = u(\omega)a^Q(\omega), \tag{3.12}$$

where $a^Q(\omega)$, the absorption coefficient, is given by

$$a^Q(\omega) = \sum_{n=0}^{\infty} p_n \times\left[\sum_{k>n} B_{nk}\delta(\omega - \omega_{kn}) - \sum_{k<n} B_{nk}\delta(\omega - \omega_{nk})\right], \tag{3.13}$$

B_{nk} being the Einstein coefficients for absorption (if $n<k$) and stimulated emission (if $n>k$), which are known to coincide for the same pair of states. To order λ, only $k = n \pm 1$ contribute and we get

$$a^Q(\omega) = \sum_{n=0}^{\infty} p_n[B_{n+1}\delta(\omega - \omega_{n+1}) - B_n\delta(\omega - \omega_n)], \tag{3.14}$$

where we have written B_n and ω_n for $B_{n,n-1}$ and $\omega_{n,n-1}$, respectively. From the well known relation of the Einstein A and B coefficients we get

$$a^Q(\omega) = \sum_{n=1}^{\infty} a_n^Q \delta(\omega - \omega_n)$$

with

$$a_n^Q = \frac{4\pi^2e^2}{3\hbar}\omega_n|\langle\varphi_n|\hat{x}|\varphi_{n-1}\rangle|^2(p_{n-1} - p_n) = \frac{2\pi^2e^2\omega_n}{3m\omega_0}n(p_{n-1} - p_n) \times\left\{1 + \frac{\lambda}{\hbar\omega_0}\frac{[(V\hat{a}^{+2})_{n-2} - (V\hat{a}^{+2})_{n-1}]}{n}\right\}. \tag{3.15}$$

Finally, the total power absorbed is, to order λ,

$$W_a^Q = \frac{2\pi^2e^2}{3m}u(\omega_0) + \lambda\frac{\pi^2e^2}{3m^2\omega_0}u'(\omega_0)\langle V''\rangle_Q. \tag{3.16}$$

The system is in equilibrium with radiation if the spontaneous emission (3.8) is exactly balanced by the combined effect of absorption and stimulated emission (3.12). The condition obtained for equilibrium is that $u(\omega)$ is given by the Planck formula (without zero point) (2.20).

We must call attention to the fact that the validity of expressions (3.10) and (3.16) in general imposes restrictions to the temperature. This is because those expressions demand that the values of ω contributing to $I_e^Q(\omega)$ and $I_a^Q(\omega)$ be close enough to ω_0. Thus, if $V(x)$ increases at most as fast as x^2 when $x \to \infty$, the expressions are valid for all T. However, if $V(x)$ goes faster than x^2, that is, $\lim_{x\to\infty} V(x)/x^2 = \infty$, then the larger T the smaller λ, in such a way that some combination of λ and T must be kept small. A necessary condition can be obtained by imposing $\omega_n \simeq \omega_0$, i.e., $\lambda(V_n - V_{n-1})/\hbar\omega_0 \ll 1$ [see (3.4)]. If we consider potentials of the form $V = x^{2K}$, $K > 1$, it is enough to consider this condition for the largest values of n in which

we are interested [see (B3a)]. The maximum of a_n^Q is obtained to order zero in λ for $n_M = (\beta\hbar\omega_0)^{-1}$ [see (3.15) and (6.11)]. For high temperatures, $n_M \gg 1$, and we can apply the results of Appendix A to get [see (6.12a) with $n \sim n_M$]

$$\frac{K}{2^K}\binom{2K}{K}\frac{\lambda(k_B T)^{K-1}}{(m\omega_0^2)^K} \ll 1. \tag{3.17}$$

IV. SPONTANEOUS EMISSION IN A CLASSICAL ELECTRODYNAMICS

We consider a system described by Eq. (2.10) and we must study its emission and absorption of radiation. As in the quantum case, there is spontaneous emission associated with the damping term in (2.10) and both absorption and stimulated emission associated with the last term of (2.10). That is, the power transferred from the field to the particle, $\dot{x}E$, is sometimes positive and other times negative. Indeed, very likely this fact inspired Einstein in his theory of absorption and emission of light, but in recent times it is often stated incorrectly that the stimulated emission (and even the spontaneous emission) is a purely quantum effect.

The power spontaneously emitted per unit frequency interval can be found from a Fourier analysis of the fields produced by the charge and a calculation of the contribution to the energy due to the corresponding Fourier components obtained in that analysis. Averaging over all possible states, it is found[11] that

$$I_e^{\mathrm{cl}}(\omega) = \frac{8\pi e^2\omega^3}{3c^3}\int_0^\infty dE\,\rho(E)\sum_n \delta(\omega - n\omega(E))|x_n(E)|^2. \tag{4.1}$$

The Fourier components x_n are of order λ^n if $n > 1$, and then only x_1 contributes to order λ, a situation that corresponds to the fact that in the quantum case only the Einstein coefficients $A_{n,n-1}$ contribute to order λ [see after Eq. (3.2)]. As a difference with the quantum case, however, the Dirac delta disappears with the integral over E, and thus the spectrum is continuous [if $\rho(E)$ is continuous]. The total emitted power (integrated to all frequencies) is

$$W_e^{\mathrm{cl}} = \frac{8\pi e^2}{3c^3}\int_0^\infty dE\,\rho(E)\omega^3(E)|x_1(E)|^2. \tag{4.2}$$

It is obvious that the (continuous) spectral form of the emitted power (4.1) cannot agree with the (discrete) quantum expression. As for the integrated power, (4.2), it does not in general agree with (3.10). We are interested in the classical ensemble in equilibrium with a radiation having a spectrum $S_{\mathscr{E}}$. The distribution function $\rho(E)$ is now given by $\rho_{\mathrm{st}}(E)$, expression (2.21). The total emitted power, (4.2), can be calculated to first order in λ by making use of the expansions (2.12) and (2.14) as well as expression (2.19). The result is given by

$$W_e^{\mathrm{cl}} = \frac{2e^2}{3mc^3}\phi(\beta\hbar\omega_0) \times\left[1 + \frac{\lambda}{2m\omega_0^2}\left(3 + \beta\hbar\omega_0\frac{\phi'(\beta\hbar\omega_0)}{\phi(\beta\hbar\omega_0)}\right)\langle V''\rangle\right], \tag{4.3}$$

where $\langle V''\rangle$ is obtained by writing (2.21) with $\omega(E) \equiv \omega_0$, namely, the harmonic oscillator. This mean value coincides with the quantum one (3.11) only if the spectrum is that of Planck with zero point. On the contrary, as concerns ϕ, (4.3) agrees with the quantum result (3.10) only if the spectrum is that of Planck without zero point.

We must call attention to the fact that the expression (4.3) is valid only if the expansions (2.12) and (2.14) are valid for the energies contributing appreciably to (4.2). Note that $\rho_{\mathrm{st}}(E)$, (2.21), is negligible for $E \gg \hbar\omega_0\,\phi(\beta\hbar\omega_0) \times(1 + O(\lambda))$. Then, if we consider potentials of the form $V = x^{2K}$, $K > 1$, the condition $\omega(E) \simeq \omega_0$ yields [see (6.2) and (6.3)],

$$\frac{K}{2^K}\binom{2K}{K}\frac{\lambda}{(m\omega_0^2)^K}[\hbar\omega_0\phi(\beta\hbar\omega_0)]^{K-1} \ll 1. \tag{4.4}$$

For high temperatures this condition is the same as the quantum one (3.17).

V. ABSORPTION AND STIMULATED EMISSION IN A CLASSICAL ELECTRODYNAMICS

The absorption of energy by a classical (stochastic) system immersed in a cavity radiation at a given temperature from an incident electromagnetic field has been calculated[12] by use of the Kubo linear response,[13] which is also based on the smallness of the parameter $\gamma = 2e^2\omega_0/3mc^3$.

This quantity in fact accounts for absorption and stimulated emission by the system and would correspond to the quantity I_a^Q calculated in Sec. III. The absorption coefficient, defined by

$$I_a^{\mathrm{cl}}(\omega) = a^{\mathrm{cl}}(\omega)u(\omega), \tag{5.1}$$

is given by[12]

$$a^{\mathrm{cl}}(\omega) = \frac{8\pi^3}{3}\omega e^2\int_0^\infty dE\,\frac{G_E}{G_{EE}}\rho(E) \times\sum_{n=-\infty}^{+\infty} n|x_n|^2\delta(\omega - n\omega(E)), \tag{5.2}$$

where

$$\frac{G_E}{G_{EE}} = \frac{2\omega^2(E)}{3\pi c^3 S_{\mathscr{E}}(\omega(E))} = \frac{1}{\hbar\omega(E)\phi(\beta\hbar\omega(E))}. \tag{5.3}$$

Again, only the $n = \pm 1$ terms contribute to order λ. By using the expansions (2.12) and (2.14) we obtain for the total absorbed power

$$W_a^{\mathrm{cl}} = \frac{2e^2\pi^2}{3m}u(\omega_0) + \lambda\frac{\pi^2e^2}{3m^2\omega_0}\langle V''\rangle u'(\omega_0) + O(\lambda^2). \tag{5.4}$$

This expression coincides with the quantum one, given by (3.16), when $\langle V''\rangle = \langle V''\rangle_Q$, that is, the spectrum of the radiation in the cavity is that of the Planck with zero point. The same expression (5.4) gives[11] the absorbed power from the radiation in the cavity by taking $u = (\hbar\omega^3/\pi^2c^3)\phi$.

We make a final remark about these results. The state described by $\rho_{\mathrm{st}}(E)$ is the stationary state corresponding to the radiation with spectrum $S_{\mathscr{E}}(\omega)$. This means that the system is in global equilibrium (equal absorbed and emitted powers) with the radiation. This equilibrium is fulfilled at all

orders in λ. Now, up to first order in λ only the frequencies close to ω_0 contribute to the emitted and absorbed powers given by (4.3) and (5.4). Consequently, these expressions must coincide, which can be easily checked by expressing $u(\omega)$ in terms of ϕ. However, there is radiative equilibrium only if the radiation in the cavity has a Rayleigh–Jeans spectrum (see Refs. 3 and 11). Note that for this equilibrium to hold, not only the global absorbed and emitted power must coincide, but also the detailed structure of the emission and absorption of energy given by $I_e^{\rm cl}(\omega)$ and $I_a^{\rm cl}(\omega)$. We finally note that a similar remark to that appearing at the end of Secs. III and IV is also applicable to the calculations in this section.

VI. SHAPE OF THE SPECTRAL ABSORPTION BANDS

In the previous sections we have compared the quantum and classical spectral line around ω_0 in what concerns the total area lying below the curves $I_a^Q(\omega)$, $I_a^{\rm cl}(\omega)$, $I_e^Q(\omega)$, and $I_e^{\rm cl}(\omega)$, that is we have compared W_a^Q, $W_a^{\rm cl}$, W_e^Q, and $W_e^{\rm cl}$. In this section we want to go further and analyze the very shape of those curves. However, we must restrict ourselves to potentials of the form

$$V=x^{2K},\quad K>1, \tag{6.1}$$

in order to get explicit results. The study of more general potentials presents special difficulties, as, for instance, that in general the function $\omega(E)$ does not have a unique solution for E and this complicates the analysis, as we shall shortly see.

We remark that for this kind of potential (6.1), the classical limit, $\beta\hbar\omega_0\to 0$, must be performed in such a way that some combination of λ and T must be kept small (see the end of Secs. III and IV).

The first information about the shape of the curves is obtained in the lowest order in λ of the expressions giving $I_a^Q(\omega)$, $I_a^{\rm cl}(\omega)$, $I_e^Q(\omega)$, and $I_e^{\rm cl}(\omega)$. Let us consider separately the classical and the quantum case. We first analyze the classical case due to its simplicity.

A. Classical case

As for the absorption, we study the shape of $a^{\rm cl}(\omega)$, which is characteristic of the system, not so $I_a^{\rm cl}(\omega)=a^{\rm cl}(\omega)\times u(\omega)$. It is easy to see in Eqs. (4.1) and (5.2) that to lowest order in λ, $I_e^{\rm cl}(\omega)$ and $a^{\rm cl}(\omega)$ are proportional. Thus their shape is similar. Let us then concentrate on $a^{\rm cl}(\omega)$.

In order to integrate over E in (5.2) we need to express E in terms of ω. For the case of (6.1), the expression (2.12) gives

$$\omega(E)=\omega_0(1+\lambda E^{K-1}T_K),\quad E>0, \tag{6.2}$$

with

$$T_K=\frac{K}{2^K}\binom{2K}{K}\frac{1}{(m\omega_0^2)^K} \tag{6.3}$$

and then

$$E=\left(\frac{\omega-\omega_0}{\lambda\omega_0 T_K}\right)^{1/(K-1)},\quad \omega\geqslant\omega_0. \tag{6.4}$$

Now we may integrate over E (recall that only the $n=1$ and $n=-1$ terms contribute). To lowest order in λ we get

$$a^{\rm cl}(\omega)=\frac{2\pi^2e^2}{3m}\frac{1}{[\hbar\omega_0\phi(\beta\hbar\omega_0)]^2}\frac{1}{(K-1)}\times\left(\frac{1}{\omega_0\lambda T_K}\right)^{2/(K-1)}(\omega-\omega_0)^{-((K-3)/(K-1))}\times\exp\left[-\frac{(\omega-\omega_0)^{1/(K-1)}}{(\omega_0\lambda T_K)^{1/(K-1)}\hbar\omega_0\phi(\beta\hbar\omega_0)}\right], \tag{6.5}$$

when $\omega\geqslant\omega_0$, and $a^{\rm cl}(\omega)=0$ when $\omega<\omega_0$.

It will be convenient to distinguish three cases, namely, $K=2$, $K=3$, and $K>3$. For $K=2$ we have

$$a^{\rm cl}(\omega)=\frac{2\pi^2e^2}{3m}\left(\frac{m^2\omega_0^3}{3\lambda}\right)^2\frac{1}{[\hbar\omega_0\phi(\beta\hbar\omega_0)]^2}(\omega-\omega_0)\times\exp\left[-\frac{(\omega-\omega_0)m^2\omega_0^3}{3\lambda\hbar\omega_0\phi(\beta\hbar\omega_0)}\right],\quad \omega\geqslant\omega_0, \tag{6.6}$$

and for $K=3$

$$a^{\rm cl}(\omega)=\frac{\pi^2e^2}{3m}\left(\frac{2m^3\omega_0^5}{15\lambda}\right)\frac{1}{[\hbar\omega_0\phi(\beta\hbar\omega_0)]^2}\times\exp\left[-\frac{\sqrt{\omega-\omega_0}}{\hbar\omega_0\phi(\beta\hbar\omega_0)}\sqrt{\frac{2m^3\omega_0^5}{15\lambda}}\right],\quad \omega\geqslant\omega_0. \tag{6.7}$$

We see that whereas for $K\geqslant 3$ the function $a^{\rm cl}(\omega)$ is always decreasing, for $K=2$, $a^{\rm cl}(\omega)$ vanishes at $\omega=\omega_0$ and has a maximum at

$$\omega_m=\omega_0+(3\lambda\hbar/m^2\omega_0)\phi(\beta\hbar\omega_0). \tag{6.8}$$

On the other hand, for $K>3$ $a^{\rm cl}(\omega)$ diverges at $\omega=\omega_0$, like $(\omega-\omega_0)^{-((K-3)/(K-1))}$, whereas for $K=3$ $a^{\rm cl}(\omega)$ tends to a finite value at $\omega=\omega_0$.

As regards the width of the curves, it can be roughly estimated from (6.5) as

$$\Delta\omega\sim\omega_0\lambda T_K[\hbar\omega_0\phi(\beta\hbar\omega_0)]^{K-1}. \tag{6.9}$$

Note that, according to (4.4), for the perturbative calculation to be valid, the width must be small, $\Delta\omega/\omega_0\ll 1$. It is also clear that condition (4.4) does not guarantee that the tail of $a^{\rm cl}(\omega)$ is correctly described by (6.5).

B. Quantum case

First of all we note that here again the expressions $I_{e,n}^Q$ and a_n^Q are proportional to each other, to the lowest order in λ. Let us then consider a_n^Q. From (3.15) we obtain

$$a_n^Q=(2\pi^2e^2/3m)(e^{\beta\hbar\omega_0}-1)^2e^{-\beta\hbar\omega_0 ne^{-n\beta\hbar\omega_0}}. \tag{6.10}$$

Now we have definite lines at the frequencies given by (3.4). We may consider that they present a "continuum" aspect when (3.5) is satisfied, that is, the width of the lines is of the order of the separation between neighbor lines. From (B3c) it is easy to see that the ratio between the width and the line separation decreases when n (and the frequency) increases for $K>3$. For $K=3$ that ratio is approximately constant if $n\gg 1$, and for $K=2$ it increases with n. When n is of order of $(\beta\hbar\omega_0)^{-1}$ and the temperature is high enough to have $\beta\hbar\omega_0\ll 1$, we can use the results of Appendix A to get

$$\omega_n \simeq \omega_0 [1 + \lambda T_K (n\hbar\omega_0)^{K-1}] \tag{6.11a}$$

and

$$\omega_n - \omega_{n-1} \simeq \omega_0 \lambda T_K (\hbar\omega_0)^{K-1} n^{K-2}(K-1). \tag{6.11b}$$

Then, for frequencies such that $1 \ll n \lesssim (\beta\hbar\omega_0)^{-1}$ (or smaller when $K>3$) the spectrum can be considered continuous when the following condition is satisfied:

$$\frac{4}{3}\frac{k_B T}{mc^2}\left(\frac{e^2}{\hbar c}\right) \gtrsim [\lambda T_K (k_B T)^{K-1}] \frac{\hbar\omega_0}{k_B T}(K-1). \tag{6.12}$$

Taking into account condition (3.17), it is clear that (6.12) can be satisfied in the region $\hbar\omega_0 \ll k_B T \ll mc^2$ for high enough temperatures. For larger frequencies corresponding to $n \gg (\beta\hbar\omega_0)^{-1}$ the perturbative calculations based on (3.17), are not valid.

When (6.12) is satisfied, we may obtain the value of $a(\omega_n)$ for each line by multiplying the value a_n^Q times the density of lines in that point. The density of lines, μ_n, is related to the inverse of the line separation. There is not a unique way of defining μ_n except for the case $n \gg 1$, for then, $\omega_n - \omega_{n-1} \simeq \omega_{n+1} - \omega_n$, and we can write $\mu_n = (\omega_{n+1} - \omega_n)^{-1}$. [This can be easily seen by using (6.11b).] Now, if we define

$$a^Q(\omega_n) = a_n^Q \mu_n = a_n^Q (\omega_{n+1} - \omega_n)^{-1} \tag{6.13}$$

and write n in terms of ω_n in expression (6.12a), we get $a^Q(\omega_n)$. Using the same functional dependence for $\omega \neq \omega_n$, we have

$$a^Q(\omega) = \frac{2\pi e^2}{3m}\left(\frac{e^{\beta\hbar\omega_c}-1}{\hbar\omega_0}\right)^2 e^{-\beta\hbar\omega_0}\frac{1}{(K-1)} \times \left(\frac{1}{\omega_0 \lambda T_K}\right)^{2/(K-1)} (\omega-\omega_0)^{-((K-3)/(K-1))} \times \exp\left[-\frac{(\omega-\omega_0)^{1/(K-1)}\beta}{(\lambda\omega_0 T_K)^{1/(K-1)}}\right], \quad \omega > \omega_0, \tag{6.14}$$

where T_K is given by (6.3).

According to the discussion above, this expression is valid only when $\omega \simeq \omega_n$ such that $1 \ll n \lesssim (\beta\hbar\omega_0)^{-1}$. We must then consider high temperatures, and in this case (6.14) is exactly accounted for by the classical expression (6.5).

As concerns the rest of the shape, a qualitative analysis can be made distinguishing again the three cases, $K=2$, $K=3$, and $K>3$.

For $K=2$ the problem is trivial because the separation between lines is constant and then

$$a^Q(\omega_n) = a_n^Q/(\omega_{n+1} - \omega_n).$$

An explicit calculation gives finally

$$n = (\omega - \omega_n)/12(\lambda/\hbar)(\hbar/2m\omega_0)^2$$

and

$$a^Q(\omega) = \frac{2\pi^2 e^2}{3m}\left(\frac{e^{\beta\hbar\omega_0}-1}{\hbar\omega_0}\right)^2 e^{-\beta\hbar\omega_0}\left(\frac{m^2\omega_0^3}{3\lambda}\right)^2 (\omega-\omega_0) \times \exp\left[-\frac{(\omega-\omega_0)m^2\omega_0^3\beta}{3\lambda}\right], \tag{6.15}$$

which has the same qualitative behavior as the classical expression (6.6) and coincides with it in the case of high enough temperatures.

For $K \geqslant 3$ there is no unique way of defining μ_n. A reasonable definition arises taking certain average between the separation on the right and on the left. Thus, for $K=3$ the choice

$$\mu_n = [a(\omega_n - \omega_{n-1}) + (1-a)(\omega_{n+1} - \omega_n)]^{-1}, \quad 0 \leqslant a \leqslant 1$$

gives

$$\mu_n = \frac{m^3\omega_0^3}{15\lambda\hbar^2}\frac{1}{n + (\frac{1}{2} - a)}$$

and

$$a^Q(\omega) = \frac{\pi^2 e^2}{3m}\left(\frac{e^{\beta\hbar\omega_0}-1}{\hbar\omega_0}\right)^2 e^{-\beta\hbar\omega_0}\left(\frac{2m^3\omega_0^5}{15\lambda}\right) \times \frac{1}{1 + (\frac{1}{2}-a)\left[2\left(\frac{\omega-\omega_0}{\xi} - 1\right)\right]^{-1/2}} \times \exp\left[-\sqrt{\frac{\omega-\omega_0}{\xi} - 1}\,\frac{\beta\hbar\omega_0}{\sqrt{2}}\right], \quad \omega \geqslant \omega_0 + \xi, \tag{6.16}$$

with

$$\xi = 15\lambda\hbar^2/4m^3\omega_0^3. \tag{6.17}$$

It is easy to see that the result is very close to the classical one (6.7) for high temperatures when the frequency is such that $\omega - \omega_0 \gg \xi$. Note that $\omega_0 + \xi$ is the first frequency observed in the quantum case. Moreover the concept of line density loses its meaning for the first line.

If we perform the classical limit $\beta \to 0$, in such a way that (3.17) holds, we verify that $a^Q(\omega)$ and $a^{cl}(\omega)$ coincide for any frequency.

For the case $K \geqslant 4$ we easily see that the situation gets more complicated. Anyway it is possible to show that the curve is everywhere decreasing, if the line density is defined by averaging the separation to the right and to the left, that is,

$$\mu_n = [a(\omega_n - \omega_{n-1}) + (1-a)(\omega_{n+1} - \omega_n)]^{-1}, \quad 0 \leqslant a \leqslant 1. \tag{6.18}$$

We only need to show that

$$n\mu_n - (n+1)\mu_{n+1} > 0, \quad \forall n \geqslant 2, \quad \forall K \geqslant 4. \tag{6.19}$$

If we call $\Delta_n = \omega_n - \omega_{n-1}$, the above inequality is satisfied if the relations

$$\Delta_{n+1} > \Delta_n > \cdots > \Delta_2 > 0, \quad n\Delta_{n+2} - (n+1)\Delta_{n+1} > 0, \quad \forall n \geqslant 1, \quad K \geqslant 4, \tag{6.20}$$

hold. Such inequalities are proved in Appendix B and then we deduce that with the above choice for μ_n, the curve $a^Q(\omega)$ is everywhere decreasing and thus has a qualitative behavior similar to the classical curve. As we have shown above, both curves coincide for high temperatures if we consider frequencies large enough for the assymptotic expression (6.11a) to be valid. For the case $K=3$, we have seen that this happens when $\omega - \omega_0 \gg \xi$. This restriction can be

expressed for the general case in the following way [see (6.11a)]:

$$(\omega-\omega_0)/\lambda\omega_0 T_K(\hbar\omega_0)^{K-1}\gg 1. \tag{6.21}$$

In the classical limit combined with condition (3.17) (i.e., $T\to\infty$, $\lambda\to 0$, and λT^{K-1} fixed but small) this restriction disappears, and $a^Q(\omega)$ coincides with $a^{cl}(\omega)$ for any frequency.

VII. DISCUSSION

We have compared the quantum and the classical anharmonic oscillators immersed in cavity radiation at a finite temperature. As is well known, the radiation in equilibrium with the system has a Planck spectrum in the quantum case and a Rayleigh–Jeans spectrum in the classical one. As expected, we have found that in all cases the quantum and the classical behavior approach each other as the temperature increases. We have also considered the classical system immersed in a radiation having a Planck spectrum with zero point, and we have shown that its behavior is much closer to the quantum one than the purely classical case (i.e., the system immersed in radiation with Rayleigh–Jeans spectrum). This is the most interesting result of our calculations. For the sake of simplicity we shall label QED the first system, CED (for classical electrodynamics) the second one, and SED (for stochastic electrodynamics) the oscillator immersed in Planck's radiation with zero point. Of course, there is not detailed balance in SED, i.e., there is not an equilibrium at each frequency, but the oscillator can be stationary if it is inside a very large cavity.

In Sec. II, we have calculated the average energy of the anharmonic oscillator and found that there is agreement to *first order in λ at all temperatures* between *QED and SED [compare Eq. (2.9) with (2.22)]* taking $\phi=\phi_{PC}$ given in (2.20). In contrast, both results agree with CED (2.4) only at high temperatures. The agreement between SED and QED disappears at second order in λ, as has been shown elsewhere for zero temperature.

In Secs. III–V, we have compared the power emitted and absorbed globally (i.e., summed to all frequencies). Again CED agrees with either QED and SED only at high temperatures. In contrast, much closer results are obtained in the comparison of QED and SED. The spontaneously emitted power in SED [see Eq. (4.3)] does not agree with the QED result (3.10) because the function ϕ of the former corresponds to the complete Planck spectrum (i.e., including zero point) and the later to the incomplete one. However, it is not possible to put in the SED (4.3) result the incomplete Planck spectrum because then the average $\langle V''\rangle$ does not agree. Indeed, as discussed above, averages in SED must be calculated with the complete spectrum. However, it is easy to realize that agreement exists at all temperatures and first order in λ between SED and QED if we subtract in the former the zero point contribution. However, the stationary average values must be always calculated including the zero point field. The absorption and stimulated emission is given by (3.16) for QED and (5.4) for SED. Indeed, both expressions are formally identical. However, it should be noted, as before, that $\langle V''\rangle$ in (5.4) should be calculated for the system immersed in radiation with the complete Planck equation. Then, the net power absorbed (i.e., after subtraction of the stimulated emission) is *identical to first order in λ* for an arbitrary incoming radiation in QED and SED. No agreement should be expected at higher orders in λ as the stationary values already do not agree.

So far so good for the total power emitted or absorbed. However, the spectral distribution is sharply different in the quantum (QED) and both classical (CED and SED) cases. In fact, the former is a discrete spectrum whilst the latter are continuous. In every case there are absorption and emission bands at ω_0, $2\omega_0$, etc. Each band is resolved in lines in the quantum case. These lines have a natural width which becomes of the order of the distances between neighbor lines for small anharmonicities [see Eq. (3.5)] and also for high temperatures, even if the potential increases faster than x^2 [see condition (6.12)].

We have made a comparison of the shape of the bands (or "bunches" of lines) in Sec. VI for anharmonic perturbations of the type λx^{2K} ($K=2,3,\ldots$). Now the agreement between QED and SED exists only at high temperatures. This agreement holds for any frequency when $K=2$ [compare Eqs. (6.6) and (6.15)] and only for large enough frequencies when $K\geqslant 3$. This restriction disappears in the classical limit, $\hbar\omega_0/k_B T\to 0$.

In conclusion, we found that SED gives results much closer to QED than purely classical electrodynamics, very close indeed in some cases. However, it is shown again that both theories are certainly not identical.

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APPENDIX A: ASYMPTOTIC EXPRESSION FOR ω_n

For a potential λx^{2K}, the frequencies ω_n appearing in the quantum emission and absorption are to first order in λ

$$\omega_n=\omega_0\left[1+\frac{\lambda}{\hbar\omega_0}\left(\frac{\hbar}{2m\omega_0}\right)^K \times\left(\langle n|(\hat a+\hat a^+)^{2K}|n\rangle-\langle n-1|(\hat a+\hat a')^{2K}|n-1\rangle\right)\right]. \tag{A1}$$

We want to calculate this expression for large n.

In the mean value of $(\hat a+\hat a^+)^{2K}$, only those terms having the same number of creation as annihilation operators contribute. Each term gives after reordering a polynomial in the number operator $\hat N=\hat a^+\hat a$, in such a way that both the higher power appearing is K and its coefficient is the unit. Moreover we have $\binom{2K}{K}$ terms like that. All this means that

$$\langle n|(\hat a+\hat a^+)^{2K}|n\rangle=\sum_{j=0}^{K} a_j^{(K)} n^j,\quad a_K^{(K)}=\binom{2K}{K}. \tag{A2}$$

Now, for large n, only the first term appearing in (A2) is important

$$\langle n|(\hat a+\hat a^+)^{2K}|n\rangle\simeq\binom{2K}{K} n^K \tag{A3}$$

and then

$$\langle n|(\hat{a}+\hat{a}^+)^{2K}|n\rangle - \langle n-1(\hat{a}+\hat{a}^+)^{2K}|n-1\rangle$$
$$\simeq \binom{2K}{K}(n^K-(n-1)^K)\simeq Kn^{K-1}\binom{2K}{K}, \qquad \text{(A4)}$$

which leads to expression (6.11a).

APPENDIX B: PROOF OF EQS. (6.20)

Let us define, by induction,

$$\phi^{(0)}_{k,n} = \langle n|(\hat{a}+\hat{a}^+)^{2k}|n\rangle, \quad n\geqslant 0, \qquad \text{(B1a)}$$
$$\phi^{(r)}_{k,n} = \phi^{(r-1)}_{k,n} - \phi^{(r-1)}_{k,n-1}, \quad n\geqslant r>0. \qquad \text{(B1b)}$$

It is obvious that

$$\Delta_n = (\lambda/\hbar)(\hbar/2m\omega_0)^K \phi^{(2)}_{K,n} \qquad \text{(B2)}$$

and then, the positivity of Δ_n and the relations (6.20) are equivalent to showing

$$\phi^{(2)}_{k,n}>0, \quad n\geqslant 2, \qquad \text{(B3a)}$$
$$\phi^{(3)}_{k,n}>0, \quad n\geqslant 3, \qquad \text{(B3b)}$$
$$n\phi^{(2)}_{k,n+2} - (n+1)\phi^{(2)}_{k,n+1}>0, \quad n\geqslant 1, \quad k\geqslant 4. \qquad \text{(B3c)}$$

In fact we shall prove (B3c) and

$$\phi^{(r)}_{k,n}>0, \quad n\geqslant r, \quad \forall r. \qquad \text{(B3d)}$$

To do this, let us define the following operators acting upon the quantities $\phi^{(r)}_{k,n}$:

$$\delta\phi^{(r)}_{k,n} = \phi^{(r)}_{k,n+1} - \phi^{(r)}_{k,n} \equiv \phi^{(r+1)}_{k,n+1}, \quad n\geqslant r, \qquad \text{(B4a)}$$

$$E\phi^{(r)}_{k,n} = \phi^{(r)}_{k,n+1}, \quad n\geqslant r. \qquad \text{(B4b)}$$

The following relations are immediate:

$$\phi^{(r)}_{k,n} = E^{n-r}\phi^{(r)}_{k,r}, \quad n\geqslant r, \qquad \text{(B5a)}$$
$$\delta^j\phi^{(r)}_{k,r} = \phi^{(r+j)}_{k,r+j}, \qquad \text{(B5b)}$$
$$E = 1+\delta. \qquad \text{(B5c)}$$

They allow us to write

$$\phi^{(r)}_{k,n} = E^{n-r}\phi^{(r)}_{k,r} = (1+\delta)^{n-r}\phi^{(r)}_{k,r} = \sum_{j=0}^{n-r}\binom{n-r}{j}\delta^j\phi^{(r)}_{k,r}$$
$$= \sum_{j=0}^{n-r}\binom{n-r}{j}\phi^{(r+j)}_{k,r+j}. \qquad \text{(B6)}$$

Now, let us define the quantities

$$\zeta_{n,k,m} = \frac{(k+m)!n!}{(n+m)!k!}\langle n(\hat{a}+\hat{a}^+)^k(\hat{a}^+)^m|n\rangle. \qquad \text{(B7)}$$

An easy calculation yields

$$\zeta_{n,k,m} - \zeta_{n-1,k,m} = \zeta_{n-1,k-1,m+1}, \qquad \text{(B8)}$$

and from the definitions (B1) we get

$$\phi^{(r)}_{k,n} = \begin{cases}\zeta_{n-r,2k-r,r}, & r\leqslant 2k,\\ 0, & r>2k,\end{cases} \qquad \text{(B9)}$$

and particularly

$$\phi^{(r)}_{k,r} = \begin{cases}\zeta_{0,2k-n,n}, & n\leqslant 2k,\\ 0, & n>2k.\end{cases} \qquad \text{(B10)}$$

Consequently, from (B6)

$$\phi^{(r)}_{k,n} = \sum_{\substack{j=0\\ j\leqslant 2k-r}}^{n-r}\binom{n-r}{j}\zeta_{0,2k-r-j,r+j}. \qquad \text{(B11)}$$

The positivity of $\phi^{(r)}_{k,n}$ for all $n\geqslant r$ will be guaranteed if all the quantities $\langle 0|(a+a^+)^k(a^+)^m|0\rangle$ are shown to be nonnegative for all k,m.

Those quantities are obviously nonvanishing only in the case that $m\leqslant k$ and both integers have the same parity.

By making use of the recurrence relation

$$\langle 0|(\hat{a}+\hat{a}^+)^k(\hat{a}^+)^m|0\rangle$$
$$= m\langle 0|(\hat{a}+\hat{a}^+)^{k-1}(\hat{a}^+)^{m-1}|0\rangle$$
$$+ (k-1)\langle 0|\hat{a}+\hat{a}^+)^{k-2}(\hat{a}^+)^m|0\rangle, \qquad \text{(B12)}$$

it is easy to obtain

$$\langle 0|(\hat{a}+\hat{a}^+)^k(\hat{a}^+)^m|0\rangle$$
$$= \frac{k!}{(k-m)!!}, \quad m\leqslant k, \quad m+k \text{ even}. \qquad \text{(B13)}$$

With this, from (B7), (B11) can be written as

$$\phi^{(r)}_{k,n} = \sum_{\substack{j=0\\ j\leqslant k-r}}^{n-r}\binom{n-r}{j}\frac{(2k)!}{(r+j)!(2k-2r-2j)!!}, \qquad \text{(B14)}$$

expressions which are clearly positive. This proves (B3d). To prove (B3c) we make an explicit calculation

$$n\phi^{(2)}_{k,n+2} - (n+1)\phi^{(2)}_{k,n+1}$$
$$= \sum_{\substack{j=0\\ j\leqslant k-2}}^{n}\binom{n}{j}\frac{(2k)!n}{(j+2)!(2k-4-2j)!!}$$
$$- \sum_{\substack{j=0\\ j\leqslant k-2}}^{n-1}\binom{n-1}{j}\frac{(2k)!(n+1)}{(2+j)!(2k-4-2j)!!}$$
$$= \frac{(2k)!n}{(n+2)!(2k-4-2n)!!}$$
$$+ \sum_{\substack{j=0\\ j\leqslant k-2}}^{n-1}\frac{(2k)!}{(j+2)!(2k-2j-4)!!}$$
$$\times\left[n\binom{n}{j} - (n+1)\binom{n-1}{j}\right], \qquad \text{(B15)}$$

where the first term exists only if $n\leqslant k-2$.

All terms in that expression are positive except for the $j=0$ term.

However, the contribution of both $j=0$ and $j=1$ gives

$$\frac{n\binom{n}{1} - \binom{n-1}{1}(n+1)}{3!(2k-6)!!} + \frac{n\binom{n}{0} - \binom{n-1}{0}(n+1)}{2!(2k-4)!!}$$
$$= \frac{1}{2(2k-6)!!}\left[\frac{1}{3} - \frac{1}{2k-4}\right], \qquad \text{(B16)}$$

which is positive for $k\geqslant 4$. This finally proves (B3c).

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Direct calculation of the Berry phase for spins and helicities

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The Berry phase for spins or helicities is calculated in a simple way in which it appears more as a property of the spin states than of the Hamiltonian. The calculation applies to nonrelativistic particles or relativistic particles with either zero or nonzero mass. A simple way to see how the Berry phase corresponds to rotation of the electric and magnetic fields of plane-polarized light is also pointed out.

I. INTRODUCTION

The Berry phase[1] that is the object of experiments recently proposed[2] and reported[3] is for spins or helicities. For these cases it can be calculated more simply, in some respects, than it was[1] originally. I do that here in a way that brings out some fundamental aspects. One is that the Berry phase appears more as a property of the spin states than of the Hamiltonian. Another is that it makes no difference whether the particle with spin is nonrelativistic or relativistic or whether it has zero or nonzero mass. I also point out a simple way to see how the Berry phase corresponds to rotation of the electric and magnetic fields of plane-polarized light.

After the first version of this paper was finished and sent, I received a paper[4] by Bialynicki-Birula and Bialynicki-Birula in which the Berry phase is obtained from the action of the Poincaré group on the states of relativistic particles with spin or helicity. We use different methods but get the same results and take a similar point of view that gives more attention to the spin states than to the Hamiltonian.

II. BASIS

I repeat the first few steps of Berry's calculation[1] to clarify the assumptions that need to be made, point out that the spin states play a bigger role than the Hamiltonian, and set the stage for arguing that the calculation applies equally well to nonrelativistic particles or relativistic particles with either zero or nonzero mass. Consider a particle spin represented by matrices $\mathbf{S}$. For each real three-vector $\mathbf{k}$ let $\hat{k}$ be the unit vector in the direction of $\mathbf{k}$. Then $\hat{k}\cdot\mathbf{S}$ represents the projection of the spin in that direction. Let $|\hat{k}\cdot\mathbf{S}=m\rangle$ be normalized eigenvectors of $\hat{k}\cdot\mathbf{S}$ for the eigenvalues m with phases chosen to make the vectors differentiable as functions of $\mathbf{k}$. For example, they can be obtained by making rotations with the spin matrices from the standard eigenvectors for $\hat{k}$ in the z direction.

Suppose the evolution of spin states in time is governed by a time-dependent Hamiltonian $H(t)$ so that at each time t there is a $\mathbf{k}(t)$ such that $|\hat{k}(t)\cdot\mathbf{S}=m\rangle$ for fixed m is an eigenvector of $H(t)$ with eigenvalue $E_m(t)$,

$$H(t)|\hat{k}(t)\cdot\mathbf{S}=m\rangle=E_m(t)|\hat{k}(t)\cdot\mathbf{S}=m\rangle.$$

Then one possible state, which could be realized as adiabatic evolution caused by a slowly changing Hamiltonian, is represented by

$$|\psi(t)\rangle=e^{-i\omega_m(t)}e^{i\gamma_m(t)}|\hat{k}(t)\cdot\mathbf{S}=m\rangle,$$

where ω_m and γ_m are real functions of t and

$$\frac{d}{dt}\omega_m(t)=E_m(t).$$

We are not assuming anything about the phase of this state vector. The Schrödinger equation

$$i\frac{d}{dt}|\psi(t)\rangle=H(t)|\psi(t)\rangle$$

implies

$$\frac{d}{dt}\gamma_m(t)=i\,\nabla\langle\hat{k}(t)\cdot\mathbf{S}=m|\hat{r}\cdot\mathbf{S}=m\rangle|_{\mathbf{r}=\mathbf{k}(t)}\cdot\frac{d}{dt}\mathbf{k}(t),$$

where ∇ is the gradient with respect to $\mathbf{r}$.

Suppose that in the time between $t=0$ and $t=T$ the vector $\mathbf{k}(t)$ moves around a closed loop C in three-dimensional space so that

$$\mathbf{k}(0)=\mathbf{k}(T).$$

If

$$|\psi(0)\rangle=|\hat{k}(0)\cdot\mathbf{S}=m\rangle$$

then

$$|\psi(T)\rangle=e^{-i\omega_m(T)}e^{i\gamma_m(C)}|\hat{k}(0)\cdot\mathbf{S}=m\rangle,$$

where

$$\omega_m(T)=\int_0^T E_m(t)dt$$

and

$$\gamma_m(C)=i\int_C\nabla\langle\hat{k}\cdot\mathbf{S}=m|\hat{r}\cdot\mathbf{S}=m\rangle|_{\mathbf{r}=\mathbf{k}}\cdot d\,\mathbf{k}.$$

Evidently $\omega_m(T)$ comes from the dynamics. It depends on the Hamiltonian. The remaining phase $\gamma_m(C)$, the Berry phase, comes from $\mathbf{k}(t)$ moving around the closed loop C. It does not depend on how that is made to happen; it does not depend on the Hamiltonian. It appears simply as an integral around C. We can also write it as an integral over a surface S enclosed by C,

$$\gamma_m(C)=i\int_S\nabla_2\times\nabla_1\langle\hat{r}_2\cdot\mathbf{S}=m|\hat{r}_1\cdot\mathbf{S}=m\rangle|_{\mathbf{r}_1=\mathbf{k}=\mathbf{r}_2}\cdot d\,\mathbf{S},$$

using gradients ∇_1 and ∇_2 with respect to $\mathbf{r}_1$ and $\mathbf{r}_2$. No further consideration of the Hamiltonian is needed.

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III. SIMPLIFICATION

It is from this point that the calculation is simplified. Let

$$\hat{k}' = R(\theta)\hat{k},$$

where $R(\theta)$ means rotation through the angle $|\theta|$ around the axis in the direction of θ. Then

$$\hat{k}'\cdot\mathbf{S} = \hat{k}\cdot\mathbf{R}^{-1}(\theta)\mathbf{S} = e^{-i\theta\cdot\mathbf{S}}\hat{k}\cdot\mathbf{S}e^{i\theta\cdot\mathbf{S}}$$

so $e^{-i\theta\cdot\mathbf{S}}|\hat{k}\cdot\mathbf{S} = m\rangle$ is an eigenvector of $\hat{k}'\cdot\mathbf{S}$ for the eigenvalue m. Then

$$|\hat{k}'\cdot\mathbf{S} = m\rangle = e^{i\beta_m(\hat{k},\theta)}e^{-i\theta\cdot\mathbf{S}}|\hat{k}\cdot\mathbf{S} = m\rangle,$$

with β_m a real function of $\hat{k}$ and θ. If

$$\mathbf{k}' = \mathbf{k} + \Delta\mathbf{k},$$

then to first order in $\Delta\mathbf{k}$

$$\begin{aligned}|\hat{k}'\cdot\mathbf{S} = m\rangle &= e^{i\alpha_m(\hat{k})\cdot\Delta\mathbf{k}}e^{-ik^{-2}\mathbf{k}\times\Delta\mathbf{k}\cdot\mathbf{S}}|\hat{k}\cdot\mathbf{S} = m\rangle \\ &= |\hat{k}\cdot\mathbf{S} = m\rangle \\ &\quad + i(\alpha_m(\hat{k}) + k^{-2}\mathbf{k}\times\mathbf{S})\cdot\Delta\mathbf{k}|\hat{k}\cdot\mathbf{S} = m\rangle,\end{aligned}$$

with α_m a real three-vector function of $\hat{k}$, so

$$\nabla|\hat{r}\cdot\mathbf{S} = m\rangle|_{\mathbf{r}=\mathbf{k}} = i(\alpha_m(\hat{k}) + k^{-2}\mathbf{k}\times\mathbf{S})|\hat{k}\cdot\mathbf{S} = m\rangle$$

and

$$\begin{aligned}\nabla_2\times\nabla_1\langle\hat{r}_2\cdot\mathbf{S} = m|\hat{r}_1\cdot\mathbf{S} = m\rangle|_{\mathbf{r}_1=\mathbf{k}=\mathbf{r}_2} &= \langle\hat{k}\cdot\mathbf{S} = m|(\alpha_m(\hat{k}) + k^{-2}\mathbf{k}\times\mathbf{S}) \\ &\quad\times(\alpha_m(\hat{k}) + k^{-2}\mathbf{k}\times\mathbf{S})|\hat{k}\cdot\mathbf{S} = m\rangle \\ &= k^{-4}\mathbf{k}\langle\hat{k}\cdot\mathbf{S} = m|\mathbf{k}\cdot\mathbf{S}\times\mathbf{S}|\hat{k}\cdot\mathbf{S} = m\rangle \\ &= ik^{-4}\mathbf{k}\langle\hat{k}\cdot\mathbf{S} = m|\mathbf{k}\cdot\mathbf{S}|\hat{k}\cdot\mathbf{S} = m\rangle \\ &= imk^{-2}\hat{k}.\end{aligned}$$

Thus we can see that

$$\gamma_m(C) = -m\Omega(C),$$

where $\Omega(C)$ is the solid angle of vectors $\mathbf{k}$ enclosed by C. Since $\nabla\cdot r^{-2}\hat{r}$ is zero everywhere except at the origin we can see the surface integral for $\gamma_m(C)$ is not changed if the surface S is changed without bringing it across the origin of the $\mathbf{k}$ vectors.

IV. RANGE OF APPLICATIONS

It is remarkable that for each nonzero spin eigenvalue m, any phase factor $e^{i\gamma}$ can be obtained from some solid angle Ω. This provides a wealth of opportunities for interference effects. In particular, for photons, when m is ± 1, the phase factor -1 is obtained when Ω is π, for example when C is the circle made by a vector $\mathbf{k}(t)$ that revolves around an axis at a 60° angle from the axis. Thus it is particularly interesting to see that the calculation made here applies to relativistic particles with zero mass.

In fact the calculation applies equally well to nonrelativistic particles or relativistic particles with either zero or nonzero mass. From the Foldy form for irreducible unitary representations of the Poincaré group[5] we can see that for relativistic particles with mass the matrices and states for spin and helicity are the same as for nonrelativistic particles. By using a basis of helicity eigenvectors[6] we can see that the spin and helicity matrices and their eigenvectors are not changed when the mass goes to zero.[7] When the mass is zero there are only two possible helicity states for a particle but they are part of a (possibly larger) space where all the spin matrices and eigenvectors are the same as for a particle with mass.[7] Since each Berry phase is for one helicity state, the formula for the Berry phase that holds when the mass is not zero must continue to hold when the mass is zero.

In the clearest experiment reported so far,[3] the Berry phase measured is an angle of rotation of a plane of polarization of light. Here is a simple way to see how changing the helicity states of photons by Berry phases corresponds to rotating the electric and magnetic fields $\mathbf{E}$ and $\mathbf{B}$. The field operators $\mathbf{B} + i\mathbf{E}$ contain only creation operators for photons with helicity $+1$ and annihilation operators for photons with helicity -1 so a change of photon states for helicity ± 1 by phase factors $e^{\mp i\Omega}$ caused by Berry phases

$$\gamma_{\pm 1}(C) = \mp\Omega$$

has the same effect on matrix elements of the field operators as a change of field operators that gives

$$\mathbf{B} + i\mathbf{E} \to e^{i\Omega}(\mathbf{B} + i\mathbf{E}),$$

which is equivalent to

$$\mathbf{B} \to \mathbf{B}\cos\Omega - \mathbf{E}\sin\Omega, \quad \mathbf{E} \to \mathbf{E}\cos\Omega + \mathbf{B}\sin\Omega.$$

This is observed[3] as rotation of the plane of polarization.

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Compatibility of observables represented by positive operator-valued measures

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The proof of a result analogous to that in Koelman and de Muynck [Phys. Lett. A **98**, 1 (1983)] is given for the case of unbounded observables. If two, not necessarily bounded, observables are represented by a positive operator-valued measure, then the measurement of any of them is undisturbed if and only if they commute. The Naimark theorem on dilations of spectral functions is exploited. A stronger version of Wigner's theorem is given.

I. INTRODUCTION

It has been shown in Ref. 1 that the commutation of two observables can be implied by a kind of minimum principle. However, the proof given in Ref. 1 is valid only for bounded s.a. operators with discrete spectrum. In the present paper we prove an analogous result, without this restriction.

II. UNIQUENESS OF THE ORTHOGONAL SPECTRAL MEASURES

We start with a simple observation that the Kadison inequality for dilations can be extended for unbounded operators in the following sense.

Lemma 1: Let B be an unbounded s.a. operator in a Hilbert space H, let P be the orthogonal projection onto a Hilbert subspace H_1 of H, and let $A = PBP$ be a s.a. operator on H_1. Then for every $f \in D(A^2) \cap D(PB^2P)$,

$$(f|A^2 f) \leqslant (f|PB^2Pf).$$

Proof: We have $P \leqslant 1$, thus for all $g \in D(B^2)$

$$(Bg|PBg) \leqslant \|Bg\|^2 = (g|B^2 g).$$

For $h \in D(BPB) \cap D(B^2)$ we have

$$(h|BPBh) \leqslant (h|B^2 h).$$

Hence, for $f \in D(A^2) \cap D(PB^2P)$ [then $f \in D(BP)$], $Pf \in D(B^2) \cap D(BPB)$. Putting $h = Pf$, we have $h \in D(BPB)$, and thus

$$(f|(PBP)^2 f) \leqslant (f|PB^2Pf). \qquad \square$$

In a symbolic way we write

$$(PBP)^2 \leqslant PB^2P.$$

With the same notation as in Lemma 1 we have the following lemma.

Lemma 2: Let P be an orthogonal projection and B a s.a. operator. Then

$$(PBP)^2 = PB^2P \tag{1}$$

if and only if P commutes with B (i.e., P commutes with the spectral projections of B).

Proof: If P commutes with B, then obviously (1) holds.

Conversely, let (1) hold. Then $D(A^2) = D(PB^2P)$, where, as before $A = PBP$ is a s.a. operator. Let E denote the spectral measure of A and let Δ be a bounded Borel set in $\mathbb{R}^1$. Denote $A_\Delta = E(\Delta)AE(\Delta) = AE(\Delta)$. Then A_Δ is a bounded s.a. operator in H_1. Further, we have

$$A_\Delta = E(\Delta)PBPE(\Delta) = E(\Delta)BE(\Delta),$$

since $E(\Delta) \leqslant P = 1_{H_1}$. Thus the operator $E(\Delta)BE(\Delta)$ is bounded for every bounded Borel set Δ in $\mathbb{R}^1$. By the assumption we have

$$A_\Delta{}^2 = PE(\Delta)B^2E(\Delta)P$$
$$= E(\Delta)B^2E(\Delta) = (E(\Delta)BE(\Delta))^2,$$

that is, for every $f \in H$,

$$(f|E(\Delta)B^2E(\Delta)f) = \|BE(\Delta)f\|^2 = \|E(\Delta)BE(\Delta)f\|^2,$$

and thus $BE(\Delta)f = E(\Delta)BE(\Delta)f$.

Obviously, for every $n = 1,2,...$, we have

$$B^nE(\Delta)f = B^{n-1}E(\Delta)BE(\Delta)f$$
$$= \cdots = E(\Delta)B^nE(\Delta)f = A^nE(\Delta)f.$$

Because for all bounded Borel sets Δ and all $f \in H$ the vectors $E(\Delta)f$ are analytic for the operator A, they are also analytic for the operator B. The set $\{E(\Delta)f | f \in H, \Delta \text{ bounded Borel}\}$ is dense in H_1. Thus, by the standard argument, for every $t \in \mathbb{R}^1$, we have

$$e^{itB}E(\Delta) = E(\Delta)e^{itB}P.$$

It follows that B commutes with all spectral projections of A, and, in particular, with the projection P. $\square$

As a corollary to the above lemmas we have the following proposition.

Proposition 1: Let A be an unbounded s.a. operator in a Hilbert space H, and let M be a positive operator-valued (POV) measure over the real line $\mathbb{R}^1$. Suppose that $A = \int \lambda M(d\lambda)$, where the integral converges strongly on the domain $D(A)$ of A (see Refs. 2–4). Then for every $f \in D(A^2)$

$$A^2 f = \int \lambda^2 M(d\lambda) f \tag{2}$$

if and only if M is an orthogonal spectral measure, i.e., it is a projection-valued measure over $\mathbb{R}^1$.

Proof: By the Naimark theorem[2,3] for any POV measure M there exists a Hilbert space H_0, such that $H \subset H_0$, and a projection-valued measure E_0 over $\mathbb{R}^1$, such that E_0 is the dilation of M by means of the projection P: $H_0 \to H$, i.e., for

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every $\Delta\subset\mathbf{R}^1$, $M(\Delta)=PE_0(\Delta)P$. Defining $B=\int\lambda E_0(d\lambda)$, we have $A=PBP$. Applying Lemma 2, we obtain

$$M(\Delta)=PE_0(\Delta)P=E_0(\Delta)P=E(\Delta),$$

for all Borel sets Δ in $\mathbf{R}^1$, where E is the orthogonal spectral measure of the operator A. Thus the POV measure M is identical with the spectral measure of A. □

III. THE MINIMAL SPREADING PRINCIPLE

Suppose now that A represents an unbounded observable associated with a physical system Σ. Thus we can assume that A is an unbounded s.a. operator in a Hilbert space H, affiliated with the von Neumann algebra $\mathfrak{A}$ generated by bounded observables verifiable in the system Σ. This means that all the spectral projections of A belong to the algebra $\mathfrak{A}$. Without loss of generality we can assume that $\mathfrak{A}$ is a factor. The states of the system are represented by probability measures on the lattice of orthogonal projections of $\mathfrak{A}$. By the generalized Gleason theorem[5] such measures are given by normal linear states on $\mathfrak{A}$. If $f\in D(A)$, then the integral $\int\lambda\mu_f(E_A(d\lambda))$ is well defined for the probability measure $\mu_f(Q)=(f|Qf)$, where E_A is the spectral measure of the operator A. Following this we say that a probability measure μ over the lattice of projections $\mathfrak{A}^P$ of the algebra $\mathfrak{A}$ is affiliated with the domain of A if the integral

$$\mu(A)=\int\lambda\mu(E_A(d\lambda)) \tag{3}$$

is convergent. Then we write $\mu\eta D(A)$. It is easy to see that μ can be weakly approximated by the measures $\mu_f, f\in D(A)$. It can be also shown that if $\mu\eta D(A_1)$ and $\mu\eta D(A_2)$, then $\mu(A_1+A_2)=\mu(A_1)+\mu(A_2)$.

Suppose now that $\mu\eta D(A^2)$ for a given s.a. operator A. Define

$$\sigma_0^2(A)=\mu(A^2)-\mu(A)^2. \tag{4}$$

Suppose further that there exists a POV measure M over the real line, such that

$$A=\int\lambda M(d\lambda), \tag{5}$$

where the integral converges strongly. Let us write formally

$$\sigma_M^2(A)=\int\lambda^2\mu(M(d\lambda))-\left(\int\lambda\mu(M(d\lambda))\right)^2.$$

Although we formulate the following results in full generality for any $\mu\eta D(A)$, it is enough to consider only measures μ_f, with $f\in D(A)$. Therefore, we omit the proofs of the following lemmas, which in the case of the measures μ_f are trivial.

Lemma 3: For every $\mu\eta D(A)$ the integral $\int\lambda\mu(M(d\lambda))$ exists and is equal to $\mu(A)$.

Lemma 4: If for two s.a. operators A_1 and A_2, we have $A_1\leqslant A_2$, then for every probability measure $\mu\eta D(A_1)\cap D(A_2)$ the following inequality holds:

$$\mu(A_1)\leqslant\mu(A_2).$$

By Lemma 1 we have always

$$A^2\leqslant\int\lambda^2M(d\lambda)=PB^2P$$

(see notation in Sec. II). Thus, for every $\mu\eta D(A^2)$, we have the inequalities of Jensen type: $\sigma_M^2(A)\geqslant 0$, and $\sigma_0^2(A)\geqslant 0$. Moreover, by Lemmas 3 and 4, the spreading is positive,

$$\delta(A)=\sigma_M^2(A)-\sigma_0^2(A)=\int\lambda^2\mu(M(d\lambda))-\mu(A^2)\geqslant 0.$$

Thus we are ready to prove the following result.

Proposition 2: For a given observable A and for every state $\mu\eta D(A^2)$ the infimum of the values of $\sigma_M^2(A)$ for all possible POV measures M is achieved on the spectral measure E_A of A, i.e., $\delta(A)=0$ if and only if $M=E_A$.

Proof: If $M=E_A$, then, obviously, $\sigma_0^2(A)=\sigma_M^2(A)$ and $\delta(A)=0$.

Conversely, if $\delta(A)=0$, then, in particular, for every $f\in D(A^2)$ [we should assume $D(A^2)=D(PB^2P)$]

$$0=\mu_f(PB^2P)-\mu_f((PBP)^2)=\mu_f(PB^2P-(PBP)^2).$$

Since, by Lemma 1, $(PBP)^2\leqslant PB^2P$ in $D(A^2)\cap D(PB^2P)$, then $PB^2Pf=(PBP)^2f$, for $f\in D(A^2)$. [$D(PB^2P)$ is dense in H, cf. Ref. 2.] Hence, by Proposition 1, it follows that $M=E_A$. □

IV. INCOMPATIBLE OBSERVABLES

Finally, we apply the results obtained above to couples of observables which possess joint POV distributions.

Lemma 5: Two (not necessarily bounded) observables A and C have a joint POV probability distribution M over $\mathbf{R}^2$ [i.e., M is a POV measure over $\mathbf{R}^2$, such that $M(\mathbf{R}^2)=1$, $A=\int\lambda M(d\lambda\times\mathbf{R}^1)$, and $C=\int\gamma M(\mathbf{R}^1\times d\gamma)$], if and only if there exists a Hilbert space H_0 and two strongly commuting s.a. operators A_0 and C_0 in H_0, respectively, such that $A=PA_0P$ and $C=PC_0P$, where P is the orthogonal projection $P: H_0\to H$.

Proof: By a straightforward extension of the Naimark theorem[2] onto the case of $\mathbf{R}^2$ there exists a Hilbert space H_0 such that the POV measure M has a dilation to an orthogonal spectral measure E_0 over $\mathbf{R}^2$, with respect to the projection $P: H_0\to H$. Since the marginal measures $E_0(\mathbf{R}^1\times\cdot)$ and $E_0(\cdot\times\mathbf{R}^1)$ are projection valued, then the operators $A_0:=\int\lambda E_0(d\lambda\times\mathbf{R}^1)$ and $C_0:=\int\gamma E_0(\mathbf{R}^1\times d\gamma)$ are s.a. operators and mutually commuting. The result easily follows. □

Proposition 3: Let A and C be two observables in the system Σ which have a joint POV probability distribution M. Suppose that for every state $\mu\eta D(A^2)$ of the system Σ we have $\sigma_0^2(A)=\sigma_M^2(A)$. Then A and C commute.

Proof: By Lemma 5 there exists a Hilbert space H_0, such that $H\subset H_0$, and A and C can be dilated to two commuting operators A_0 and C_0 in H_0. By Proposition 2, it follows from the assumption that

$$E_A=M(\cdot\times\mathbf{R}^1).$$

It is easy to see that since for all Borel sets Δ, $\Delta'\subset\mathbf{R}^1$,

$$E_0(\Delta\times\mathbf{R}^1)E_0(\mathbf{R}^1\times\Delta')=E_0(\mathbf{R}^1\times\Delta')E_0(\Delta\times\mathbf{R}^1),$$

and

$$E_A(\Delta)=E_0(\Delta\times\mathbf{R}^1)P,$$

we have

$E_A(\Delta)f \in D(C)$ and $CE_A(\Delta)f = E_A(\Delta)Cf$

for every $f \in D(C)$.

In particular, by the argument similar to that in Lemma 2 concerning analytic vectors, we get the commutation of $E_A(\Delta)$ with the spectral projections of the operator C. Thus A and C commute. □

Proposition 3 is a stronger version of Proposition 6.1, Chap. II, in Ref. 3. There the commutativity is derived from the minimal spreading of both observables. In the above Proposition 3 one of the marginal distributions can be a genuine POV measure, not necessarily a projection-valued one.

The above result can be interpreted as follows. In orthodox quantum mechanics only observables corresponding to mutually commuting self-adjoint operators are believed to be jointly measurable. The Naimark theorem, as exploited in Lemma 5, permits us to extend the notion of joint measurability to so-called incompatible observables which correspond to noncommuting s.a. operators. Thus, the joint measurement of A_0 and C_0 described in Lemma 5 can be interpreted as a joint measurement of A and C, with

$$M(d\lambda \times \mathbb{R}^1) = PE_0(d\lambda \times \mathbb{R}^1)P,$$

$$M(\mathbb{R}^1 \times d\gamma) = PE_0(\mathbb{R}^1 \times d\gamma)P.$$

It follows that two incompatible observables are jointly measurable whenever they have a joint POV probability distribution in the sense of Lemma 5. The question whether any pair of incompatible observables allows a joint POV probability distribution, and, hence, is jointly measurable, is not discussed here. For the position $\hat{q}$ and momentum $\hat{p}$ many examples are well known.[3,6,7]

The notion of a POV measure makes it possible to give a generalized definition of a quantum mechanical measurement of incompatible observables. Our present results extend the results of Ref. 1 onto the general case of unbounded observables, including position and momentum. It has been demonstrated that it is possible to measure jointly these observables only when a mutual disturbance is allowed, affecting the second (and higher) moments of both distributions. As a corollary to this result we prove a stronger version of Wigner's theorem.[8,9]

Corollary 1: There is no phase-space representation of quantum mechanics which satisfies all of the following three requirements: (i) the distribution function $f(q,p)$ on $\mathbb{R}^2$ of a state with the density operator ρ is the expectation value of a s.a. operator $M(q,p)$ (defining a POV measure over $\mathbb{R}^2$), i.e.,

$$f(q,p) = \mathrm{Tr}[\rho M(q,p)];$$

(ii) $f(q,p) \geqslant 0$;

and (iii) either

$$\int_{-\infty}^{\infty} f(q,p)dp = (q,\rho q) \tag{6}$$

or

$$\int_{-\infty}^{\infty} f(q,p)dq = (p,\rho p).$$

Proof: The impossibility of the phase-space representation is implied by Proposition 3, because the operators $\hat{q} = \int qM(q,p)dq\,dp$, and $\hat{p} = \int pM(q,p)dq\,dp$ would commute if the conditions (i)–(iii) were satisfied. □

Notice that in the previous version of Wigner's theorem[8,9] both conditions in (iii) are required. A similar result was obtained by Twareque Ali and Prugovečki[10] under the additional hypothesis of covariance under the Galilean group.

Corollary 2: (iii)′ The operator which corresponds to a phase-space function of the form $A(q) + B(p)$, where $A(q)$ and $B(p)$ are arbitrary Borel functions, is $A(\hat{q}) + B(\hat{p})$, thus

$$A(\hat{q}) + B(\hat{p}) = \int \{[A(q) + B(p)]M(q,p)\}dq\,dp \tag{7}$$

implies both conditions in (iii), and hence, it is not a weaker condition, as assumed in Ref. 9.

Proof: According to Proposition 1, in order to prove (6), it is sufficient to take $A(q) = 1, q$, and q^2, and $B(p) = 0$ in (7). □

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Heisenberg inequality and the complex field in quantum mechanics

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Observables A and B satisfy the Heisenberg inequality if the product of their variances has a positive lower bound independent of the state of the system. In the Hilbert space formulation of quantum mechanics it is a consequence of the Schwarz inequality that the Heisenberg-type inequality $\mathrm{Var}(A,\varphi)\cdot\mathrm{Var}(B,\varphi)\geqslant\frac{1}{4}|\langle A\varphi\,|B\varphi\rangle-\langle B\varphi\,|A\varphi\rangle|^2$ holds for any pair of observables A and B (represented as self-adjoint operators) and for any (vector) state (represented as a unit vector). If $\inf\{|\langle A\varphi\,|B\varphi\rangle-\langle B\varphi\,|A\varphi\rangle|\;|\varphi\in\mathrm{dom}(A)\cap\mathrm{dom}(B)\}\neq 0$ then A and B satisfy the Heisenberg inequality. In the present paper the derivability of the Heisenberg-type inequality is analyzed within the general theoretical frame of a sum logic. It is shown that any real-valued non-negative function $(A,\alpha)\to f(A,\alpha)$ of observables A and of states α, which has a symmetry property $f(A+B,\alpha)+f(A-B,\alpha)=2f(A,\alpha)+2f(B,\alpha)$ with respect to observables, satisfies the Heisenberg-type inequality $f(A,\alpha)\cdot f(B,\alpha)\geqslant\frac{1}{4}|f(A+B,\alpha)-f(A,\alpha)-f(B,\alpha)|^2$ for all observables A and B and for all states α. The natural probabilistic realizations $f_1(A,\alpha)=\mathrm{Exp}(A^2,\alpha)$ and $f_2(A,\alpha)=\mathrm{Var}(A,\alpha)$ of such functions are then analyzed. It turns out that only with the complex extension of the theory can the Heisenberg inequality be attained in the Hilbert space realization of the theory. This is used as an argument in favor of the complex field as the scalar field of quantum mechanics.

I. INTRODUCTION

Since the discovery of the fundamental "exchange relation" $QP-PQ=(ih/2\pi)I$ and the uncertainty relation $\Delta Q\cdot\Delta P\geqslant h/4\pi$ in the early days of quantum mechanics the problems of interpretation and derivability of these relations have constituted one of the central issues on the foundations of the theory. In this paper we do not touch the problem of interpretation of the uncertainty relation but we attempt to investigate the question of under which conditions two observables satisfy the probabilistic uncertainty relation. As we wish to avoid here the problems of interpretation we refer to the uncertainty relation in the sequel more neutrally as the Heisenberg inequality. We shall now introduce our problem in more detail.

Heisenberg inequalities characterize pairs of observables for which the product of their variances has a positive lower bound independent of the state of the system. The existence of such pairs of observables is characteristic for quantum systems. Observables A and B are said to satisfy the *Heisenberg inequality* if there is a positive number h, say, such that

$$\mathrm{Var}(A,\alpha)\cdot\mathrm{Var}(B,\alpha)\geqslant h \tag{1}$$

holds for any state α of the system. Here, e.g., $\mathrm{Var}(A,\alpha)$ denotes the variance of A in the state α. If A and B satisfy the Heisenberg inequality (1) then, in particular, they are unbounded, noncompatible, and even totally noncompatible. These results do not depend on the structure of the Hilbert space quantum mechanics but are valid also in more general theories.[1–3]

In the Hilbert space quantum mechanics, where observables are represented as self-adjoint operators in a (complex, separable) Hilbert space $\mathbf{H}$ and (pure) states as unit vectors (modulo phase factors) of $\mathbf{H}$, one derives the inequality

$$\mathrm{Var}(A,\varphi)\cdot\mathrm{Var}(B,\varphi)\geqslant\tfrac{1}{4}|\langle A\varphi\,|B\varphi\rangle-\langle B\varphi\,|A\varphi\rangle|^2, \tag{2}$$

which holds for any pair of observables A and B and for any state $\varphi\in\mathbf{H}$ in the intersection $\mathrm{dom}(A)\cap\mathrm{dom}(B)$ of the domains of A and B.[4] Here $\langle\cdot|\cdot\rangle$ denotes the inner product of $\mathbf{H}$. The inequality (2) follows essentially from the Schwarz inequality. The number $\frac{1}{4}|\langle A\varphi\,|B\varphi\rangle-\langle B\varphi\,|A\varphi\rangle|^2$ gives now one possible estimate for the lower bound of the product $\mathrm{Var}(A,\varphi)\cdot\mathrm{Var}(B,\varphi)$. Thus if

$$\inf\{|\langle A\varphi\,|B\varphi\rangle-\langle B\varphi\,|A\varphi\rangle|\;|\varphi\in\mathrm{dom}(A)\cap\mathrm{dom}(B)\}\neq 0,$$

then A and B satisfy the Heisenberg inequality. In particular, if A and B are such that their commutator $AB-BA$ equals to a scalar operator cI, $|c|\neq 0$, on a dense subspace $\mathbf{D}$ of $\mathbf{H}$, then

$$\inf\{|\langle A\varphi\,|B\varphi\rangle-\langle B\varphi\,|A\varphi\rangle|\;|\varphi\in\mathbf{D}\}=|c|.$$

However, as $\mathbf{D}\subset\mathrm{dom}(AB)\cap\mathrm{dom}(BA)$ might be contained properly in $\mathrm{dom}(A)\cap\mathrm{dom}(B)$, $|c|$ need not give a lower bound for $\mathrm{Var}(A,\varphi)\cdot\mathrm{Var}(B,\varphi)$, with $\varphi\in\mathrm{dom}(A)\cap\mathrm{dom}(B)$. This fact reflects the importance of the distinction between the Schrödinger and Heisenberg couples (see Garrison and Wong[5]; for examples demonstrating the above conclusion see, e.g., Lahti,[1] Beltrametti and Cassinelli,[2] or Lahti and Ylinen[6]). For Schrödinger couples the right-hand side of (2) does give a positive lower bound leading thus to the Heisenberg inequality (1).

We shall now turn to analyze the derivability of the Heisenberg-type inequality (2) in a general quantum logic frame and discuss the relevance of the complex field to the Heisenberg inequality (1).

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II. DERIVATION OF AN ABSTRACT HEISENBERG-TYPE INEQUALITY

In this section $\mathbf{E}$ is a real vector space.

Definition 2.1: A *quadratic functional* on $\mathbf{E}$ is any function $f: \mathbf{E}\to\mathbb{R}$ that is non-negative [i.e., $f(x)\geqslant 0$ for all $x\in\mathbf{E}$] and has the property

$$f(x+y)+f(x-y)=2f(x)+2f(y) \quad \text{for all } x,y\in\mathbf{E}. \tag{3}$$

Theorem 2.2: Any quadratic functional $f: \mathbf{E}\to\mathbb{R}$ satisfies the inequality

$$f(x)\cdot f(y)\geqslant \tfrac{1}{4}|f(x+y)-f(x)-f(y)|^2 \quad \text{for all } x,y\in\mathbf{E}. \tag{4}$$

Proof: Note first that $f(0)=0$. We shall now define $h(x,y):=\frac{1}{2}(f(x+y)-f(x)-f(y))$ for all $x,y\in\mathbf{E}$, and note that h is additive with respect to the first variable, i.e., $h(x+z,y)=h(x,y)+h(z,y)$ for all $x,y,z\in E$. As h is symmetric, h is also additive with respect to the second variable. Now it easily follows that $h(2x,y)=2h(x,y)$, and, by induction, that $h(nx,y)=nh(x,y)$ for any natural number $n\in\mathbb{N}$. We also have $h(-nx,y)=-nh(x,y)$ and, with substituting $nx=z$, we obtain $h((1/n)x,y)=(1/n)h(x,y)$. Hence $h(qx,y)=qh(x,y)$ for any rational number q. Putting now $x=y$ in Eq. (3) of Definition 2.1 we obtain $f(2x)=4f(x)$. By a similar argument as above we infer that $f(qx)=q^2f(x)$ for any rational number q. Now for fixed $x,y\in\mathbf{E}$, $x\neq 0$, we define p: $\mathbb{R}\to\mathbb{R}$ with $p(q)=f(qx+y)=2h(qx,y)+f(qx)+f(y)$. As p is non-negative we have $0\leqslant q^2f(x)+2qh(x,y)+f(y)$ for all rational numbers q. Being a quadratic polynomial in q, p is a continuous function of q for fixed $x,y\in\mathbf{E}$. Thus the inequality $0\leqslant q^2f(x)+2qh(x,y)+f(y)$ holds for all real numbers q. Hence the discriminant must be nonpositive, so that $|h(x,y)|^2\leqslant f(x)\cdot f(y)$ for all $x,y\in\mathbf{E}$. For $x=0$ this is evident. This completes the proof.

Remark 2.3: The proof of the theorem does not depend on the choice of the number field of $\mathbf{E}$. Thus it holds also when $\mathbf{E}$ is a complex vector space.

Remark 2.4: If $h: \mathbf{E}\times\mathbf{E}\to\mathbb{R}$ is a symmetric [i.e., $h(x,y)=h(y,x)$ for all $x,y\in\mathbf{E}$] bilinear (i.e., linear with respect to both arguments) form, then the quadratic form $f(x):=h(x,x)$, $x\in\mathbf{E}$, associated with h is a quadratic functional. Conversely, any quadratic functional f which is hemicontinuous at $0\in\mathbf{E}$ [i.e., $\lim_{n\to\infty}(\lambda_n x)=0$ for any sequence $(\lambda_n)\subset\mathbb{R}$ for which $\lim_{n\to\infty}\lambda_n=0$] defines a symmetric bilinear form $h(x,y):=\frac{1}{2}(f(x+y)-f(x)-f(y))$, $x,y\in\mathbf{E}$, such that $f(x)=h(x,x)$, $x\in\mathbf{E}$, i.e., f is a quadratic form.[7]

The existence of a quadratic functional on a given vector space $\mathbf{E}$ is by no means obvious. In some probabilistic applications the existence of such functionals is, however, crucial. In the following we shall distinguish a class of quantum logics on which quadratic functionals can be defined. To do that we shall first recall the relevant notions and terminology. In that we follow the presentation of Beltrametti and Cassinelli.[2]

Let $(\mathbf{L},\mathbf{S})$ be a quantum logic, where $\mathbf{L}$ is an orthomodular, σ-orthocomplete partially ordered set and $\mathbf{S}$ is a sufficient set of states (i.e., generalized probability measures) on $\mathbf{L}$. Let $\mathbf{B}(\mathbb{R})$ denote the Borel σ-algebra of the real line $\mathbb{R}$. An observable A is a σ-homomorphism $\mathbf{B}(\mathbb{R})\to\mathbf{L}$. Any pair (A,α) of an observable A and a state α defines a (standard) probability measure μ_α^A: $\mathbf{B}(\mathbb{R})\to[0,1]$, $X\mapsto\mu_\alpha^A(X):=\alpha(A(X))$. Let ι be the identity function on $\mathbb{R}$. The integral $\int_{\mathbb{R}}\iota\, d\mu_\alpha^A$ is denoted as $\mathrm{Exp}(A,\alpha)$ and it is called the expectation value of the observable A in the state α. Similarly, $\mathrm{Exp}(A^2,\alpha)$ and $\mathrm{Var}(A,\alpha)$ denote the second moment and variance of A in the state α, respectively. An observable A is said to be bounded if its spectrum (or support) $\mathrm{sp}(A):=\cap\{X\in\mathbf{B}(\mathbb{R})\mid X \text{ is closed, and } A(X)=e\}$ is bounded. (Here e denotes the unit element of $\mathbf{L}$.) A quantum logic $(\mathbf{L},\mathbf{S})$ is said to be a sum logic, if the sum $A+B$ of any two bounded observables A and B exists and is unique; $A+B$ is then defined through the formula

$$\mathrm{Exp}(A+B,\alpha):=\mathrm{Exp}(A,\alpha)+\mathrm{Exp}(B,\alpha) \quad \text{for all } \alpha\in\mathbf{S}.$$

For any $\lambda\in\mathbb{R}$, λA is an observable defined through $\mathrm{Exp}(\lambda A,\alpha)=\lambda\,\mathrm{Exp}(A,\alpha)$ for all $\alpha\in\mathbf{S}$. Thus, in a sum logic $(\mathbf{L},\mathbf{S})$, the set $\mathbf{O}$ of all bounded observables forms a real vector space.

Definition 2.5: Let $(\mathbf{L},\mathbf{S})$ be a sum logic and $\mathbf{O}$ the set of bounded observables on it. $(\mathbf{L},\mathbf{S})$ is a *quadratic logic* if there exists a real function f on the Cartesian product $\mathbf{O}\times\mathbf{S}$ such that $f(\cdot,\alpha)$ is a quadratic functional for any $\alpha\in\mathbf{S}$.

In the next section we shall show that there are quadratic logics. Before going into that we obtain, as a corollary to Theorem 2.2, that quadratic logics are distinguished in that an abstract Heisenberg-type inequality holds true in them.

Corollary 2.6: Let $(\mathbf{L},\mathbf{S})$ be a quadratic logic, and let f: $\mathbf{O}\times\mathbf{S}\to\mathbb{R}$ be such a function that $f(\cdot,\alpha)$ is a quadratic functional for each $\alpha\in\mathbf{S}$. The following *abstract Heisenberg-type inequality* now holds true,

$$f(A,\alpha)\cdot f(B,\alpha)\geqslant\tfrac{1}{4}|f(A+B,\alpha)-f(A,\alpha)-f(B,\alpha)|^2 \tag{5}$$

for all $A,B\in\mathbf{O}$ and for any $\alpha\in\mathbf{S}$.

Let $(\mathbf{L},\mathbf{S})$ be a quadratic logic. The interpretation of the measure μ_α^A defined by a pair (A,α) as the probability measure of the possible values of the observable A in the state α suggests that natural candidates for functions f: $\mathbf{O}\times\mathbf{S}\to\mathbb{R}$ for which the inequality (5) of Corollary 2.6 could hold were among $f_0(A,\alpha):=\mathrm{Exp}(A,\alpha)$, $f_1(A,\alpha):=\mathrm{Exp}(A^2,\alpha)$, and $f_2(A,\alpha):=\mathrm{Var}(A,\alpha)$. Clearly, f_0 is out of the question (as it is linear with respect to both arguments). As concerns f_1 and f_2 they both are non-negative functions. In general, however, it is not known whether they would give rise to quadratic functionals $\mathbf{O}\to\mathbb{R}$. But as

$$f_1(A-\mathrm{Exp}(A,\alpha),\alpha)=\mathrm{Exp}(A^2,\alpha)-\mathrm{Exp}(A,\alpha)^2$$
$$=\mathrm{Var}(A,\alpha)=f_2(A,\alpha)$$

for all $A\in\mathbf{O}$, $\alpha\in\mathbf{S}$, one immediately recognizes that $f_1(\cdot,\alpha)$, $\alpha\in\mathbf{S}$, is a quadratic functional exactly when $f_2(\cdot,\alpha)$, $\alpha\in\mathbf{S}$, is such. Assuming that this were the case we would obtain the following two realizations of the abstract Heisenberg-type inequality of Corollary 2.6:

$$\mathrm{Exp}(A^2,\alpha)\cdot\mathrm{Exp}(B^2,\alpha)$$
$$\geqslant\tfrac{1}{4}|\mathrm{Exp}((A+B)^2,\alpha)-\mathrm{Exp}(A^2,\alpha)-\mathrm{Exp}(B^2,\alpha)|^2,$$

$$\mathrm{Var}(A,\alpha)\cdot\mathrm{Var}(B,\alpha)$$
$$\geq \tfrac{1}{4}|\mathrm{Var}(A+B,\alpha)-\mathrm{Var}(A,\alpha)-\mathrm{Var}(B,\alpha)|^2,$$
for all $A,B\in\mathbf{O}$, $\alpha\in\mathbf{S}$.

III. HILBERT SPACE REALIZATION

We shall now demonstrate the existence of quadratic logics by using the Hilbert space realization of the quantum logic scheme of Sec. II. In that realization the basic sets $\mathbf{L}$ and $\mathbf{S}$ are identified with the sets $\mathbf{P}(\mathbf{H})$ and $\mathbf{T}_s(\mathbf{H})_1^+$ of (orthogonal) projection operators P and positive normalized trace class operators T on the underlying Hilbert space $\mathbf{H}$. The identification of $\mathbf{S}$ with $\mathbf{T}_s(\mathbf{H})_1^+$ follows from Gleason's theorem (see, e.g., Beltrametti and Cassinelli[2]), provided that the vector space dimension of $\mathbf{H}$ is at least 3. Here we assume that this is the case. According to the spectral theorem of self-adjoint operators, each observable E^A: $\mathbf{B}(R)\to\mathbf{P}(\mathbf{H})$ can now be identified with a self-adjoint operator A in $\mathbf{H}$. Thus the set $\mathbf{O}$ of bounded observables can be identified with the set $\mathbf{L}_s(\mathbf{H})$ of bounded self-adjoint operators on $\mathbf{H}$. Actually, the results of this section can be extended in a straightforward manner to unbounded observables, as well. But to avoid the complications with the domains of the definitions of the self-adjoint operators we consider here only bounded observables.

We consider again the functions f_1 and f_2 of Sec. II, now defined on $\mathbf{L}_s(\mathbf{H})\times\mathbf{T}_s(\mathbf{H})_1^+$. As the operator product is distributive over the operator sum, the functionals $A\mapsto f_1(A,T)=\mathrm{Exp}(A^2,T)=\mathrm{tr}(TA^2)$ and $A\mapsto f_2(A,T)=\mathrm{Var}(A,T)=\mathrm{tr}(TA^2)-\mathrm{tr}(TA)^2$ are quadriatic on $\mathbf{L}_s(\mathbf{H})$ for any $T\in\mathbf{T}_s(\mathbf{H})_1^+$. Here, e.g., $\mathrm{tr}(TA^2)$ denotes the trace of TA^2 (which is a trace class operator). This shows that there are quadratic logics in the sense of Definition 2.5.

We formulate this result as a theorem,

Theorem 3.1: Let $\mathbf{H}$ be a Hilbert space whose dimension is at least 3. The pair $(\mathbf{P}(\mathbf{H}),\mathbf{T}_s(\mathbf{H})_1^+)$ is a quadratic logic. The functionals $A\mapsto\mathrm{Exp}(A^2,T)$ and $A\mapsto\mathrm{Var}(A,T)$ are quadratic functionals on $\mathbf{L}_s(\mathbf{H})$ for any $T\in\mathbf{T}_s(\mathbf{H})_1^+$, and the following Heisenberg-type inequalities hold true:

$$\mathrm{Exp}(A^2,T)\cdot\mathrm{Exp}(B^2,T)\geq\tfrac{1}{4}|\mathrm{Exp}(AB+BA,T)|^2$$
$$=\tfrac{1}{4}|\mathrm{Exp}(\{A,B\},T)|^2, \tag{6}$$
$$\mathrm{Var}(A,T)\cdot\mathrm{Var}(B,T)$$
$$\geq\tfrac{1}{4}|\mathrm{Exp}(\{A,B\}T)-2\,\mathrm{Exp}(A,T)\cdot\mathrm{Exp}(B,T)|^2, \tag{7}$$

for any $A,B\in\mathbf{L}_s(\mathbf{H})$ and for all $T\in\mathbf{T}_s(\mathbf{H})_1^+$. Here $\{A,B\}$ denote the anticommutator $AB+BA$ of A and B.

We shall next ask whether the Heisenberg-type inequalities (6) or (7) of Theorem 3.1 also serve as the Heisenberg inequalities, i.e., whether the right-hand sides of these inequalities could give a nontrivial lower bound for some pairs of observables. We shall test this with the canonically conjugate position and momentum observables Q and P, in the sense of a Schrödinger couple. We consider only one degree of freedom so that we may take $\mathbf{H}$ to be the Lebesgue space $\mathbf{L}_2(\mathbb{R})$. Consider the Gaussian state T_G which is determined by the function $\varphi_G(x)=c\exp(-ax^2)$, $x\in\mathbb{R}$, with some suitable constants a and c. In this case $\mathrm{Exp}(P,T_G)=0$ and $\mathrm{Exp}(QP,T_G)=-\mathrm{Exp}(PQ,T_G)$ so that $\mathrm{Exp}(QP+PQ,T_G)=0$. Thus, in the important case of position and momentum observables Q and P

$$\inf_{T\in\mathbf{T}_s(\mathbf{H})_1^+}|\mathrm{Exp}(\{Q,P\},T)|$$
$$=\inf_{T\in\mathbf{T}_s(\mathbf{H})_1^+}|\mathrm{Exp}(\{Q,P\},T)-2\,\mathrm{Exp}(Q,T)\cdot\mathrm{Exp}(P,T)|=0.$$

This shows that neither of the above inequalities (6) nor (7) can serve as the Heisenberg inequality for the most important pair of observables Q and P.

We shall now proceed with analyzing a complex extension of the function f_1. Let us, however, first recall that the set $\mathbf{T}_s(\mathbf{H})_1^+$ of all states is completely determined by the set $\mathrm{Ex}(\mathbf{T}_s(\mathbf{H})_1^+)$ of pure states, i.e., the extreme elements of $\mathbf{T}_s(\mathbf{H})_1^+$ which are exactly the one-dimensional projections $P[\varphi]$, φ a unit vector, on $\mathbf{H}$. If T is a mixed state, i.e., of the form $\Sigma\lambda_iP[\varphi_i]$, with $0\leq\lambda_i\leq1$, $\Sigma\lambda_i=1$, $\varphi_i\in\mathbf{H}$, then $f_1(A,T)=f_1(A,\Sigma\lambda_iP[\varphi_i])=\Sigma\lambda_if_1(A,P[\varphi_i])$, which shows that also the values of the function f_1 are determined by its values on $\mathbf{L}_s(\mathbf{H})\times\mathrm{Ex}(\mathbf{T}_s(\mathbf{H}))_1^+$. Hence, without any loss in generality but with some saving in the degree of denotational complexity, we may restrict to consider f_1 on $\mathbf{L}_s(\mathbf{H})\times\mathrm{Ex}(\mathbf{T}_s(\mathbf{H}))_1^+$, only. Observe then that

$$f_1(A,P[\varphi])=\mathrm{Exp}(A^2,P[\varphi])=\mathrm{tr}(P[\varphi]A^2)$$
$$=\langle\varphi|A^2\varphi\rangle=\langle A\varphi|A\varphi\rangle$$

for any $A\in\mathbf{L}_s(\mathbf{H})$ and for any $P[\varphi]\in\mathrm{Ex}(\mathbf{T}_s(\mathbf{H}))_1^+$. This fact proposes the following complex extension of the functions f_1:

$$\hat{f}_1\colon\ \mathbf{L}(\mathbf{H})\times\mathrm{Ex}(\mathbf{T}_s(\mathbf{H})_1^+)\mapsto\mathbb{C},$$
$$(A,P[\varphi])\mapsto\hat{f}_1(A,P[\varphi]):=\langle A\varphi|A\varphi\rangle.$$

Clearly, for any $P[\varphi]\in\mathrm{Ex}(\mathbf{T}_s(\mathbf{H})_1^+)$ the function $\hat{f}_1(\cdot,P[\varphi])$ restricted to $\mathbf{L}_s(\mathbf{H})$ agrees with the function $f_1(\cdot,P[\varphi])$. Moreover, $\hat{f}_1$ is real and it satisfies condition (3) of Definition 2.1, as well. As Theorem 2.2 holds also for complex vector spaces $\mathbf{E}$ (cf. Remark 2.3), the inequality (5) of Corollary 2.6 will also be satisfied by this function. In particular, for any two (bounded) observables A and B in $\mathbf{L}_s(\mathbf{H})$ we now have

$$f_1(A,P[\varphi])\cdot f_1(B,P[\varphi])$$
$$=\hat{f}_1(A,P[\varphi])\cdot\hat{f}_1(iB,P[\varphi])\geq\tfrac{1}{4}|\hat{f}_1(A+iB,P[\varphi])$$
$$-\hat{f}_1(A,P[\varphi])-\hat{f}_1(iB,P[\varphi])|^2$$
$$=\tfrac{1}{4}|\mathrm{Exp}(AB-BA,P[\varphi])|^2$$
$$=\tfrac{1}{4}|\mathrm{Exp}([A,B],P[\varphi])|^2,$$

where $[A,B]$ denotes the commutator $AB-BA$ of A and B. As $\mathrm{Exp}([A,B],T)$ is invariant under the scaling $A\to A-\mathrm{Exp}(A,T)$ and $B\to B-\mathrm{Exp}(B,T)$ we may rewrite the above inequality as the Heisenberg-type inequality

$$\mathrm{Var}(A,T)\cdot\mathrm{Var}(B,T)\geq\tfrac{1}{4}|\mathrm{Exp}([A,B],T)|^2, \tag{8}$$

which holds for any pair of (bounded) observables A and B and for any state T. Thus the *complex extension* $\hat{f}_1$ of f_1 allows one to derive the usual Heisenberg-type inequality (8). Though the inequality (8) is standard and well known we wish to emphasize some important features that are revealed

by the above derivation. First of all, the basic inequality (5) of Corollary 2.6 holds true in a very general setting for any quadratic functional. Second, the *natural probabilistic realization* $f_1(A,T) = \mathrm{Exp}(A^2,T)$ of such a functional does not readily lead to the Heisenberg-type inequality. Only with extending the real vector space $\mathbf{L}_s(\mathbf{H})$ of observables to the complex space $\mathbf{L}(\mathbf{H})$ and the real function f_1 to the complex one $\hat{f}_1$, one is able to derive the inequality (8). This clearly shows that the complex field is very essential for the derivability of the Heisenberg inequality (at least in the Hilbert space framework). This is remarkable as the problem of the choice of the scalar field of quantum mechanics has become very relevant, anew.[8] The Heisenberg inequality may thus serve as an argument for the choice of the complex field. In the following section we shall study the derivability of the Heisenberg-type inequality within two possible complex extensions of the abstract quantum logic framework.

IV. COMPLEX EXTENSIONS

In this section we shall investigate two possible complex extensions of an abstract quadratic logic $(\mathbf{L},\mathbf{S})$ which may allow one to derive an abstract Heisenberg inequality.

Let $(\mathbf{L},\mathbf{S})$ be a sum logic, and $\mathbf{O}$ the real vector space of bounded observables on it. We consider the function $f_1(A,\alpha) := \mathrm{Exp}(A^2,\alpha)$ on $\mathbf{O}\times\mathbf{S}$ and we assume that the functionals $A \mapsto f_1(A,\alpha)$, $\alpha\in\mathbf{S}$, are quadratic. We shall now extend the real vector space $\mathbf{O}$ to the complex one $\hat{\mathbf{O}} := \{A + iB \mid A,B\in\mathbf{O}\}$, where i is the imaginary unit. Let Φ be a bilinear $\mathbf{O}$-valued mapping on the Cartesian product $\mathbf{O}\times\mathbf{O}$ and assume that it has the property $\Phi(A,b) = \Phi(a,B) = 0$ for any constant observables $a,b\in\mathbb{R}$ [i.e., observables $\mathbf{B}(\mathbb{R})\to\mathbf{L}$ whose spectra are singletons $\{a\}$ and $\{b\}$]. We define the following function $\hat{f}_1$:

$$\hat{f}_1(A + iB,\alpha) := f_1(A,\alpha) + f_1(B,\alpha) + f_0(\Phi(A,B),\alpha)$$

for all $A,B\in\mathbf{O}$, and for any $\alpha\in\mathbf{S}$. Clearly, $\hat{f}_1$ is a real-valued function on $\hat{\mathbf{O}}\times\mathbf{S}$, whose restriction to $\mathbf{O}\times\mathbf{S}$ equals f_1. Here f_0 denotes again the expectation functional on $\mathbf{O}\times\mathbf{S}$, i.e., $f_0(\Phi(A,B),\alpha) = \mathrm{Exp}(\Phi(A,B),\alpha)$. Due to the linearity of f_0 and due to the bilinearity of Φ we obtain

$$\hat{f}_1(A + iB,\alpha) + \hat{f}_1(A - iB,\alpha) = 2\hat{f}_1(A,\alpha) + 2\hat{f}_1(B,\alpha)$$

for all $A,B\in\mathbf{O}$, $\alpha\in\mathbf{S}$. Assuming that $\hat{f}_1$ is also non-negative, we see that $\hat{f}_1(\cdot,\alpha)$ is a quadratic functional on $\hat{\mathbf{O}}$ for any $\alpha\in\mathbf{S}$. According to the complex version of Theorem 2.2 we thus have

$$\hat{f}_1(A,\alpha)\cdot\hat{f}_1(iB,\alpha) \geqslant \tfrac{1}{4}|\hat{f}_1(A + iB,\alpha) - \hat{f}_1(A,\alpha) - \hat{f}_1(iB,\alpha)|^2$$

for all $A,B\in\mathbf{O}$, $\alpha\in\mathbf{S}$. But as $\hat{f}_1(A,\alpha) = f_1(A,\alpha)$ and $\hat{f}_1(iB,\alpha) = f_1(B,\alpha)$ for all $A,B\in\mathbf{O}$, $\alpha\in\mathbf{S}$, we may rewrite this inequality in the form

$$f_1(A,\alpha)\cdot f_1(B,\alpha) \geqslant \tfrac{1}{4}|\mathrm{Exp}(\Phi(A,B),\alpha)|^2$$

for all $A,B\in\mathbf{O}$, and for all $\alpha\in\mathbf{S}$. This form of the abstract Heisenberg-type inequality, which was obtained applying the complex extension $\hat{f}_1$ of f_1, suggests that the observable $\Phi(A,B)\in\mathbf{O}$ could be interpreted as a kind of commutator of the observables A and B. We note that the "commutator" $\Phi(A,B)$ of A and B has the usual scaling invariance property $\mathrm{Exp}(\Phi(A - \mathrm{Exp}(A,\alpha),B - \mathrm{Exp}(B,\alpha)),\alpha) = \mathrm{Exp}(\Phi(A,B),\alpha)$ for any $A,B\in\mathbf{O}$, $\alpha\in\mathbf{S}$. Hence the above inequality can be rewritten once more; now in terms of the variances

$$\mathrm{Var}(A,\alpha)\cdot\mathrm{Var}(B,\alpha) \geqslant \tfrac{1}{4}|\mathrm{Exp}(\Phi(A,B),\alpha)|^2 \tag{9}$$

for all $A,B\in\mathbf{O}$, $\alpha\in\mathbf{S}$. This is simply an abstract form of the familiar Heisenberg-type inequality of the Hilbert space formulation of quantum mechanics, as given, e.g., in inequality (8) of Sec. III.

Let $(\mathbf{L},\mathbf{S})$ be a sum logic, and assume that the functionals $A \mapsto f_1(A,\alpha)$, $\alpha\in\mathbf{S}$, are quadratic on $\mathbf{O}$. It is an open question which kind of structural properties this assumption implies on $(\mathbf{L},\mathbf{S})$. We do know only that it holds true in the Hilbert space realization of the sum logic $(\mathbf{L},\mathbf{S})$. Again, in the Hilbert space model of $(\mathbf{L},\mathbf{S})$ the generalized commutator map Φ has the standard solution $\Phi(A,B) = i[A,B] = i(AB - BA)$, for $A,B\in\mathbf{L}_s(\mathbf{H})$. The problem of which kind of properties a quadratic logic $(\mathbf{L},\mathbf{S})$ has to possess in order for a nontrivial (i.e., nonzero) commutator map Φ: $\mathbf{O}\times\mathbf{O}\to\mathbf{O}$ to be constructed on it is another open problem. In general, it is known only that if $(\mathbf{L},\mathbf{S})$ admits such a nontrivial Φ and if the Heisenberg-type inequality (9) turns out to be a Heisenberg inequality for some pair of observables A and B, i.e., $\inf\{|\mathrm{Exp}(\Phi(A,B),\alpha)| \mid \alpha\in\mathbf{S}\} \neq 0$ for A and B, then these observables are totally noncommutative, and, *a fortiori*, $\mathbf{L}$ is strongly non-Boolean.[3]

There is another way of approaching the problem of generalizing the commutation relation in such a way that we obtain an abstract form of the Heisenberg inequality. Namely, we can postulate the existence of a pair of observables (a canonical pair of observables) in such a way that the right-hand side of inequality (5) in Corollary 2.6 becomes independent of A and B and has a lower bound for all states. Let $\hat{\mathbf{O}}$ be the complex vector space defined by the set $\mathbf{O}$ of (bounded) observables, and let $\hat{\mathbf{S}}$ denote the complex vector space generated by the (convex) set of state $\mathbf{S}$.[9] It then turns out that this is possible under the assumption that there is a vector space $\mathbf{X}$ and a map $g: \mathbf{X}\to\hat{\mathbf{S}}$ such that the functional $\hat{f}(A,x) := f(A,g(x))$ is quadratic not only with respect to A but also with respect to x. We then have the following theorem.

Theorem 4.1: Let $\hat{f}: \hat{\mathbf{O}}\times\mathbf{X}\to\mathbb{R}$ be a non-negative functional quadratic with respect to A and x. Assume that there is a pair of observables $A,B\in\hat{\mathbf{O}}$ such that

$$\hat{f}([A,B],cx) = \hat{f}([A,B],x) \quad \text{for all } |c| = 1 \text{ and } x\in\mathbf{X}.$$

[Here $\hat{f}([A,B],x)$ denotes $\frac{1}{4}(\hat{f}(A + B,x) - \hat{f}(A,x) - \hat{f}(B,x))$. A similar notation will be used with respect to x, as well.] If, moreover, $\hat{f}([A,B],x)$ is real-hemicontinuous at 0 with respect to x, then

$$\langle x|y\rangle := \tfrac{1}{2}\{\hat{f}([A,B],[y,x]) + i\hat{f}([A,B],[y,ix])\}$$

defines an inner product on $\mathbf{X}$ and $\|x\|^2 = \hat{f}([A,B],x)$ is a norm on $\mathbf{X}$. In this case inequality (5) of Corollary 2.6 takes the following form:

$$\hat{f}(A,x)\cdot\hat{f}(B,x) \geqslant \|x\|^4. \tag{10}$$

The proof of this theorem can be found in Maczynski.[10] If we now interpret $\hat{f}(A,x)$ as the second moment of A in the state represented by x (which is equal to the variation of centralized observables A and B, i.e., observables with zero expecta-

tion in the state represented by x), then inequality (10) takes the form

$$\mathrm{Var}(A,x)\cdot\mathrm{Var}(B,x)\geqslant\|x\|^4,$$

where $\mathrm{Var}(A,x)$ is the variance of A in the state represented by x. For states represented by normalized vectors $\|x\|=1$ the above inequality takes the form

$$\mathrm{Var}(A,x)\cdot\mathrm{Var}(B,x)\geqslant 1,$$

which corresponds to the Heisenberg inequality.

There arises a natural question of whether there exists a pair of observables satisfying the assumption of the above theorem. It turns out that in the Hilbert space model $(\mathbf{P}(\mathbf{H}),\mathbf{T}_s(\mathbf{H})_1^+)$ of the sum logic $(\mathbf{L},\mathbf{S})$ there is a realization of Theorem 4.1. In that model the set $\hat{O}$ is identified with the set $\mathbf{L}(\mathbf{H})$ of bounded operators on $\mathbf{H}$, and the set $\hat{S}$ is identified with the set $\mathbf{T}(\mathbf{H})$ of trace class operators on $\mathbf{H}$. Let the vector space $\mathbf{X}$ be the underlying Hilbert space H, and consider the function g: $\mathbf{H}\to\mathbf{T}(\mathbf{H})$, $\varphi\to g(\varphi)=P[\varphi]$. Let $\hat{f}(A,\varphi)=f(A,P[\varphi]):=\langle A\varphi\,|A\varphi\rangle$. Clearly, $\hat{f}$ is a real-valued non-negative function on $\mathbf{L}(\mathbf{H})\times\mathbf{H}$, and it is quadratic with respect to both variables. Consider now $A=iQ$ and $B=P$, where Q and P are any two self-adjoint operators in $\mathbf{H}$ such that $QP-PQ=iI$ holds in a dense subspace $\mathbf{D}$ of $\mathbf{H}$. Due to the properties of the inner product $\langle\cdot|\cdot\rangle$ of $\mathbf{H}$, the function $\hat{f}([A,B],\cdot)$ has the properties assumed in Theorem 4.1. After a straightforward calculation one obtains $\hat{f}([A,B],[\varphi,\Psi])+i\hat{f}([A,B],[\varphi,i\Psi])=2\langle\Psi|\varphi\rangle$ for any $\varphi,\Psi\in\mathbf{D}$. This shows that the inner product of $\mathbf{H}$ implied by Theorem 4.1 equals the Hilbert space inner product $\langle\cdot|\cdot\rangle$ of $\mathbf{H}$. Moreover, for any unit vector $\varphi\in\mathbf{D}$ we now have

$$\mathrm{Var}(Q,\varphi)\cdot\mathrm{Var}(P,\varphi)\geqslant 1.$$

We conclude that the usual Hilbert space realization of a sum logic gives a model of Theorem 4.1.

It is an open problem whether there exists a pair of canonical observables on a general quantum logic and what is implied by such an existence. It is quite probable that this is so strong a requirement that it already implies the usual Hilbert space formulation of quantum mechanics. In any case we see from the above consideration that to obtain a solution even in the Hilbert space we have to extend the space of observables to a complex vector space. There arises the question of why we consider the assumption about a quadratic functional (which implies the Heisenberg-type inequality for this functional) as superior to the inequality itself. The reason is that the quadracity condition is expressed as an equational axiom, and it is well known that a mathematical theory involving equational axioms only is better than a theory involving inequalities (for equational theories there are very general theorems characterizing the properties of models of these theories). We also hope that some physical motivation for the quadracity of the relevant functionals will be found. Anyway, to obtain the Heisenberg inequality it is not enough to consider only linear functionals on the vector space of observables in a sum logic. One has to bring into play a quadratic functional as well.

V. CONCLUSIONS

The problem of the choice of the number field for the mathematical apparatus of quantum mechanics has been considered by many authors. It is known that the identification of the division ring of the Piron–McLaren representation theorem with the real field $\mathbf{R}$, or with the complex field $\mathbf{C}$, or with the quaternion division ring Q is not a consequence of the lattice structure of $\mathbf{L}$ but it needs extra assumptions. These assumptions allow one to infer that the division is an extension of the real field $\mathbf{R}$,[11,12] but the selection of $\mathbf{C}$ in preference to $\mathbf{R}$ is motivated by mathematical simplicity.[2] Some more exotic fields like, e.g., p-adic numbers have been found out to be incompatible with the required lattice structure,[13] but as indicated by Beltrametti[8] the problem of giving convincing physical motivation for the choice of the complex field is still open.

In this paper the superiority of the complex field $\mathbf{C}$ over the real field $\mathbf{R}$ was demonstrated by showing that the Heisenberg inequality can be derived only in the complex field framework. If we attempt to derive this inequality from an equational axiom, we can do this only after extending the real vector space of observables to a complex one. We note that there are examples of quantum logics with a sufficient set of states satisfying the Heisenberg inequality.[1] However, in such cases the inequality is not derived but it is postulated as an axiom. Although the complex numbers do not appear directly in the Heisenberg inequality, we see that they are necessary for the derivation of it; by applying real numbers only a derivation of the Heisenberg inequality cannot be given. This is a similar situation as with the Cardano formulas for the solution of the cubic equation; even when all three roots are real, to calculate them from the real coefficients of the equation by means of Cardano's formulas we have to pass through the complex numbers. Moreover, it is known by a formal proof that without complex numbers the derivation is not possible. We hope that this analogy shows the meaning of our result. We do not claim that the complex numbers are indispensable in quantum mechanics, but we have shown that if one wants to derive the mathematical formalism of quantum mechanics with the Heisenberg inequality within the axiomatic frame of quantum logic using only equational axioms one has to pass through the complex numbers. We hope that these results may contribute towards a final solution of the problem of the number field in quantum mechanics.

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Maximal and minimal eigenvalues and their associated nonlinear equations

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The spectral theory of uniformly elliptic operators A under perturbations V giving rise to operators of the form $H_V = A + V(x)$ on a bounded or unbounded region, such as Schrödinger operators, are considered. Suppose that $\|V\|_p$ is constrained, but V is otherwise unspecified. The theory of the potentials V that maximize or minimize the eigenvalues of H_V is presented. The optimizing potentials are typically determined by equations of the form $-\Delta u + W(x)u = \pm cu^\alpha + \Lambda u$. The optimization of eigenvalues also turns out to be related to the determination of the best constants in Sobolev's inequality, and, in its one-dimensional simplification, to a classical oscillator problem with "instanton" properties.

I. INTRODUCTION

In an earlier paper,[1] one of us analyzed the following problem (the notation has been changed slightly): Let Ω be a bounded domain in $\mathbf{R}^\nu$ and consider the eigenvalue problem for various self-adjoint realizations of

$$H = -\Delta + V(x)\,. \tag{1.1}$$

Suppose that the potential V is constrained so that $\|V\|_p < M < \infty$ for some $p, 1 \leqslant p \leqslant \infty$. The earlier paper[1] characterized the potentials V subject to certain constraints of this sort that maximize the lowest eigenvalue of H_V. The predominant concern was the case $p = 1$, where the maximizers turn out to be multiples of characteristic functions, but it was noted that for $1 < p < \infty$ one was led to the nonlinear equation

$$\Delta V^{(p-1)/2} = (V - \Lambda)V^{(p-1)/2}$$

or, with

$$u = V^{(p-1)/2},\ \alpha = (p+1)/(p-1),\quad -\Delta u + u^\alpha = \Lambda u\,. \tag{1.2}$$

The key step was the realization that a necessary condition for V to be an extremizer of the functional $V \to \Lambda$, with Λ a particular eigenvalue of H_V, is that V and the associated eigenfunction u at extremum be related algebraically via

$$u^2 = c|V|^{p-1}\,. \tag{1.3}$$

The case $p = \infty$ is trivial and will henceforth be excluded. A number of questions are related to this maximizing problem either in spirit or in method. For instance, it is just as natural to ask how one could minimize an eigenvalue. Putting aside for the moment general considerations such as the existence of an extremum, the analysis of which needs somewhat different ideas from those of Ref. 1, condition (1.3) turns out to characterize minimizers as well as maximizers. Once (1.3) is derived and inserted into the variational characterization for eigenvalues, the minimizing problem becomes closely analogous to that of finding the best constant in Sobolev's inequality, a subject that has been studied extensively for its interest in the theory of elliptic partial differential equations (see Refs. 2–7). In particular, much of our work in Sec. III is directly inspired by the work of Glaser *et al.* and Lieb and Thirring (cf. Refs. 2, 3, and 6) who worked on these best constants and optimal bounds for the number of eigenvalues and their moments. Equations like (1.2) also arise in other contexts, such as the Yamabe problem of geometry, and have been reviewed by Lions.[8] More recently there has been a paper by Brézis and Nirenberg[9] bringing out more fully the connection between the general theory of equations like (1.2) and the variational techniques developed for the best constants studies.

In addition, minimization of eigenvalues arises in the mathematical physics of bulk matter and in quantum scattering theory, especially as a tool to estimate the number of bound states, i.e., negative eigenvalues of H_V on domains that may be infinite. So long as p is sufficiently large that V is relatively compact, the essential spectrum of H_V is positive, while its discrete spectrum may have negative eigenvalues bounded from below by a determinate constant, so it makes sense to speak of minimizing the eigenvalues. We have discovered that there is a body of literature on the minimizing problem on the half-line dating from papers of Everitt,[10] Eastham,[11] and Evans,[12] who produced lower bounds for the lowest eigenvalue, and culminating with the work of Veling,[13] who obtained the optimal one-dimensional lower bounds by realizing the connection with Sobolev's inequality and drawing on that literature.

We also wish to remark that in the case of one-dimensional, finite intervals there were several independent solutions (Refs. 14–17) of some maximizing problems of the type analyzed in Ref. 1. Some of them[14,16] used inequalities of the sort that are exploited for optimizing Sobolev's inequality. As a final historical note, the earliest analysis of maximal and minimal eigenvalues of the vibrating string problem of which we are aware is that of Krein,[18] who found that the optimal bounded densities constrained to have a certain L^1 norm were multiples of characteristic functions, reminiscent of a result of Ref. 1. Although some connections have been noted among all these related optimization problems, it seems that they have not been as fully recognized and

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exploited as they might have been. We are grateful to Kaper, Pranger, and Zettl for bringing some of these references to our attention.

In Sec. II we extend the analysis of Ref. 1 in certain ways, and discuss existence, uniqueness, and other properties of optimizing potentials and their associated nonlinear partial differential equations. In the last section we specialize to the case of one dimension, where the nonlinear equation can be integrated and interpreted as a problem in classical dynamics. We shall show among other things that the optimizers of the eigenvalues of H_V with different boundary conditions on a finite interval correspond to different phases of the same classical oscillator orbits. The minimizing potentials for infinite intervals are related to classical orbits with "instanton" properties, and in special cases they become familiar solitons.

II. OPTIMIZING POTENTIALS IN ν DIMENSIONS

In this section we will consider certain elliptic linear differential operators acting on a ν-dimensional Riemannian manifold Ω, for which the Rellich–Kondrashov embedding theorem[19,20] for the Sobolev spaces $W_0^{k,p}$ holds; in particular Ω can be a bounded or unbounded domain in $\mathbb{R}^\nu$ or a smooth compact manifold. The operators consist of potentials $V(x)$ added to

$$A = -\sum_{i,j} D_i a_{ij}(x) D_j + W(x) = A_1 + W(x) , \quad (2.1)$$

where A is uniformly elliptic, i.e., $a_{ij} = a_{ji}$ are absolutely continuous real functions, and for each x the eigenvalues of the matrix a_{ij} lie between (or equal) numbers a and b, $0 < a < b < \infty$. We also assume that they have bounded gradients. When W, which should be thought of as a fixed background potential, is relatively form compact (for instance, if $W \in L^p$, $p > \nu/2$, $\nu > 1$, or $p \geqslant 1$, when $\nu = 1$, cf. Refs. 21 and 22), the operator A is semibounded and self-adjoint with quadratic-form domain $W_0^{1,2} \subset L^2(\Omega)$, i.e., the operator is closed from the core of smooth functions of compact support. This corresponds to Dirichlet boundary conditions, but in Sec. III on the one-dimensional case, we shall also impose different boundary conditions. It is known that the ground-state eigenvalue of A is nondegenerate with an eigenfunction that is positive a.e., when it exists—for instance when Ω is compact.[20] (More general operator-theoretic assumptions guaranteeing this property are discussed by Reed and Simon[21] and Davies[23].) If Ω is bounded, A has a compact resolvent. For the necessary facts about elliptic operators we refer to Gilbarg and Trudinger[20] and for self-adjointness to Reed and Simon,[21] and we shall follow notation found in those references as far as possible. We shall also occasionally specialize to the most important case, $A = -\Delta$.

To the operator A will be added a real-valued function $V(x)$, called the potential, which satisfies L^p constraints, and we will consider the questions of existence, uniqueness, and characterization of the potentials that maximize or minimize a given eigenvalue, extending the results of Ref. 1 in various ways. If V is also relatively form compact, then $A + V$ has the same general properties as A. In fact, the same properties hold if the positive part of V is assumed merely L^1, except that the quadratic-form domain may be smaller.

For the case of the Laplacian on a bounded Ω and either $p = 1$ or p sufficiently large, Ref. 1 contained an existence proof for a potential V_* maximizing the lowest eigenvalue of H_V. The following is a slight generalization.

Theorem II.1: Let $\Omega \subset \mathbb{R}^\nu$ be open and bounded and, for $p > 1$, let S be a closed, convex, and bounded subset of $L^p(\Omega)$, with $V \geqslant 0$ for $V \in S$. Denote the lowest eigenvalue of $A + V$ by

$$E(V) = \inf \{(f,(A+V)f) \mid f \in W_0^{1,2}(\Omega) , \ \|f\|_2 = 1\} . \quad (2.2)$$

Then there exists a unique potential V_* in S that maximizes $E(V)$.

Proof: (1) Any maximizing sequence of V's in S contains a weakly convergent subsequence (V_n). Let $V_n \to V_*$ weakly. By a theorem of Mazur (cf. Ref. 24, p. 120), closed and convex sets are weakly closed, and so $V_* \in S$.

(2) For $\epsilon > 0$, there exists $\phi \in C_c^\infty$, $\|\phi\|_2 = 1$, such that

$$E(V_*) \geqslant (\phi,(A+V_*)\phi) - \epsilon ;$$

hence, since $V_n \to V$ weakly,

$$\epsilon + E(V_*) \geqslant (\phi,(A+V_*)\phi)$$

$$= \lim_{n\to\infty} (\phi,(A+V_n)\phi) \geqslant \limsup E(V_n)$$

by the definition of $E(V_n)$. It then follows that $E(V_*) = E_* \equiv \sup \{E(V) \mid V \in S\}$.

(3) Uniqueness of V_* follows from the strict concavity of $E(V)$: It is easy to see that $E(\cdot)$ is concave.

Suppose now that there were two maximizing potentials V_1 and V_2. By concavity their average, denoted V_3, must also be a maximizer. Denoting the corresponding normalized eigenfunctions by f_1, f_2, and f_3, we observe that unless $f_1 = f_2 = f_3$,

$$E_* = E(V_3) = I(f_3,V_3) = \tfrac{1}{2}(I(f_3,V_1) + I(f_3,V_2))$$

$$> \tfrac{1}{2}(E(V_1) + E(V_2)) = E_*$$

[here $I(f,V) \equiv (f,(A+V)f)$.] Thus $f_1 = f_2 = f_3$ and from the Schrödinger equations for f_1 and f_2 we see that $V_1 f_1 = V_2 f_2$ a.e. Since ground state eigenfunctions may be chosen to be positive in Ω, it follows that $V_1 = V_2$ a.e., and we are done. ■

For additional discussion of the case $p = 1$, see Ref. 1. The method of proof of Theorem II. 1 does not extend to other eigenvalues or to minimization even of the ground state. Theorems II.2–II.4, which use straightforward compactness arguments, are a useful replacement. The details are somewhat different for low dimensions ($\nu \leqslant 3$), because quadratic-form compactness gets one farther than operator compactness. We shall make use of the well-known Rellich–Kondrashov embedding theorem.[19,20] The space $W_0^{k,p}(\Omega)$ is compactly embedded in $L^{\nu p/(\nu - kp)}(\Omega)$ for $kp < \nu$, and in $C^m(\bar{\Omega})$ for $0 \leqslant m < k - \nu/p$.

Theorem II.2: Let $\nu = 1$, 2, or 3, and suppose Ω is bounded. Let V vary in a closed, convex, bounded set S (a) within the bounded Borel measures, if $\nu = 1$; (b) in $L^p(\Omega)$

for some $p>1$, if $\nu=2$; (c) in $L^p(\Omega)$ for some $p>\frac{3}{2}$, if $\nu=3$. Let the background potential W lie in the same class. For any fixed k, denote the kth eigenvalue of H_V by $E(V)$. Then $E(V)$ attains its maximum and minimum in S.

Proof: The proof works by throwing the emphasis not on V but on the corresponding eigenfunction, and using standard embedding theorems. The set S consists of relatively form-bounded potentials (with arbitrarily small relative bound independent of V), and the min–max principle and the Kato–Rellich theorem show that $E(V)$ is bounded above and below uniformly on S. Let E_* denote the infimum or supremum of $E(V)$ on S. Let V_n be an optimizing sequence within S, and for convenience denote the associated eigenvalue and eigenfunction E_n and g_n, $\|g_n\|_2=1$. By passing to a subsequence we may assume that $E_n\to E_*$ and that V_n converges weakly to a potential we denote $V_*\in S$. For any constant $C>E_*$, and n large,

$$C>\langle g_n,(A_1+W+V_n)g_n\rangle>(1-\epsilon)\langle g_n,A_1g_n\rangle-D,$$

for some (arbitrarily small) $0<\epsilon<1$ and some D, independent of V_n, by the uniform relative boundedness of such potentials.[21,22] The Gårding inequality then implies that there is a uniform bound on $\|\nabla g_n\|_2$, so g_n is a bounded sequence in $W_0^{1,2}$. We claim that it has a uniformly convergent subsequence by Rellich–Kondrashov. This is immediate when $\nu=1$. If $\nu=2$ we learn that g_n is bounded in L^p, all $p<\infty$, and if $\nu=3$ we attain L^p, all $p<6$. Thus, with the Hölder inequality, V_ng_n is bounded in L^p for some $p>1$ ($\nu=2$) or some $p>\frac{3}{2}$. With the assumptions on A, the same is true of Δg_n (cf. Ref. 20, Theorem 8.12, p. 186; here we must require that the boundary of Ω is of class C^2). This makes g_n bounded in $W_0^{2,p}$ for some $p>1$ when $\nu=2$, allowing us to apply the compact embedding to get the desired conclusion. If $\nu=3$, we are as yet only guaranteed $W_0^{2,6/5+\epsilon}\subset L^{6+\epsilon'}$, and a few more iterations of this argument are needed to put g_n in a sufficiently highly indexed Sobolev space to have a uniformly convergent subsequence. We call the uniform limit g_* (for $\nu=1$, 2, or 3). It is a nonvanishing element of the quadratic-form domain of A.

If g_n converges uniformly and V_n-E_n weakly,

$$(V_n-E_n)g_n\to(V_*-E_*)g_*$$

weakly, from which it is easy to see that in the distributional sense

$$(A_1+W+V_*-E_*)g_*$$

$$=\lim_n(A_1+W+V_n-E_n)g_n=0.\quad\blacksquare$$

A more abstract existence theorem makes use either of relative operator compactness or of ultracontractivity, i.e., the property that for some abstract operator B, $\exp(-tB)$ is bounded from L^2 to L^∞ for all $t>0$. A family of operators is uniformly ultracontractive if there is a uniform bound for some $t>0$. This property applies, for example, to $B+V=-\Delta+V$ acting on a bounded, smooth domain, where V is positive and ranges over some set in L^1, since $\exp(-t(B+V))$ has a kernel dominated pointwise by that of $\exp(t\Delta)$, as can be seen from the product formula.[21,25] For recent ultracontractive technology, see Refs. 22 and 26.

Theorem II.3: Let B be a positive self-adjoint operator with compact resolvent on L^2, and let V range over a convex, bounded, and closed set $S\subset L^2$. For any fixed k, we denote the kth lowest eigenvalue of $B+V$ by $E(V)$. Assume either that (a) each $V\in S$ is relatively bounded with respect to B with bound less than 1, uniformly in S; or (b) $B+V$ is self-adjoint, bounded below by a constant uniform in S, and uniformly ultracontractive for $V\in S$. Then the maximum and minimum of $E(V)$ are both attained in the set S.

Proof: As before, let V_n be a minimizing sequence, with associated eigenvalues E_n and L^2-normalized eigenfunctions g_n. We pass to a subsequence so that $E_n\to E_*$ and $V_n\to V_*$ weakly without further ado. The ultracontractive property implies a uniform bound of the form $|g_n(x)|<M$, so V_ng_n is bounded in L^2 under either assumption (a) or (b). The eigenvalue equation can be written

$$g_n=-(B+i)^{-1}(V_n-E_n-i)g_n\,. \tag{2.3}$$

Since $(V_n-E_n-i)g_n$ is bounded in L^2 and B has compact resolvent, g_n has a strong limit point, which we call g_*. As $V_n\to V_*$ weakly and $g_n\to g_*$ strongly, we have for $\phi\in C_c^\infty$

$$(V_n,g_n\phi)\to(V_*,g_*\phi)$$

implying

$$V_ng_n\to V_*g_*\quad\text{weakly},$$

as $\|V_ng_n\|\leqslant$const. This identifies the weak limit of a subsequence of $(V_n-E_n-i)g_n$. Passing to this limit, (2.3) becomes

$$g_*=-(B+i)^{-1}(V_*-E_*-i)g_*\,, \tag{2.4}$$

so g_* is an eigenfunction of $B+V_*$ with eigenvalue E_*. ■

Corollary II.4: Let Ω be bounded and have sufficiently smooth boundary (or no boundary), $A=-\Delta+W$ where $W\in L^p$, and $S=\{f\in L^p:\ \|f\|_p\leqslant M\}$ with $p>\nu/2$, $\nu\geqslant 2$ (or S is either this with $p>1$ or the set of Borel measures of total mass $\leqslant M$ if $\nu=1$). Let $E(V)$ denote the kth lowest eigenvalue of $A+V$ for fixed k. Then $E(V)$ attains its minimum in S.

Remarks about Theorems II.2–II.4: (1) The eigenvalues may be numbered by the min–max principle, counting multiplicities. Corollary II.4 for $\nu>3$ results from a standard estimate of relative boundedness given as a problem in Reed and Simon,[21] Vol. IV, p. 369 (the infinite domain there is inessential).

(2) The technique of proof often extends to show the existence of optimizers of various other spectral properties, such as gaps between eigenvalues[27] and resonance widths.[28] The one-dimensional result holds for all the boundary conditions considered in Sec. III.

(3) It is not certain how far these theorems could be extended. They certainly do not extend unchanged to dimension $\nu\geqslant 4$ and the critical value $p=\nu/2$, since by arguments like those leading to (2.11) below such an extension would imply existence of positive solutions of

$$-\Delta u=u^\alpha+\lambda u$$

for $\alpha=(\nu+2)/(\nu-2)$ and arbitrary negative λ. Yet, as noted by Brézis and Nirenberg,[9] this is not possible (at least for smooth star-shaped domains) as a consequence of the Pohozaev identity. We conjecture that ultracontractive esti-

mates might be an efficient way to study the critical values in this problem and the associated theory of nonlinear differential equations.

(4) As one would suspect from the alacrity with which we pass to subsequences in the proofs, there is no guarantee of uniqueness. In fact, some optimizing potentials are not unique (see Sec. III and Ref. 1).

Some of the natural sets of potentials over which one might wish to optimize are not convex, such as $\|V\|_p = M$. Since, however, it is easy to see from the min–max principle that any maximizer or minimizer over the set $\|V\|_p \leqslant M$ automatically has $\|V\|_p = M$, the existence Theorems II.3 and II.4 are still useful. Without loss of generality, maximizers or minimizers over these sets may be assumed *ab initio* to be non-negative and nonpositive, respectively. Hence one might also be led to consider playing the misère version of this game, viz., fix $\|V\|_p = M$ with $V \geqslant 0$ (resp. $\leqslant 0$) and attempt to minimize (resp. maximize). It turns out that there will be no minimizer under these circumstances, for the infimum of the ground state eigenvalue for A on a bounded Ω with $p > 1$, for instance, can be determined to be $E(0)$, by consideration of the sequence

$$V_n = Mn^{1/p}\chi_{B_n}, \tag{2.5}$$

where $|B_n| = 1/n$, $B_{n+1} \subset B_n \subset \Omega$. Since $V_n \to 0$ in L^1, the Rayleigh–Ritz inequality with the (bounded) ground-state eigenfunction of A as the trial function shows that

$$E(0) < E(V_n) < E(0) + \text{const}\|V_n\|_1 \to E(0).$$

Since $\|V\|_p > 0$ implies the strict inequality $E(V) > E(0)$, Theorem II.3 in fact shows that any minimizing sequence in the set considered tends weakly to 0, and thus leaves the original set. Similar but more detailed calculations show the same for $p = 1$ and for maximizing sequences of negative potentials (see Ref. 29).

In Ref. 1, uniqueness was proved for maximizers of the ground-state eigenvalue in the case $p = 1$, and one-dimensional examples were given showing that maximizers of higher eigenvalues are not unique in general. In Sec. III we arrive at some uniqueness only as a consequence of characterizing the optimizers. The uniqueness theorem for maximizers of the ground-state eigenvalue, however, can easily be extended to higher p.

Observe that minimizing potentials cannot be unique when $\Omega = R^\nu$ or any other translation-invariant domain, since translations of the potential leave the spectrum invariant.

Now that we have established the existence of at least some extrema, it remains to characterize them, along the lines of Ref. 1. Let

$$S = \{V: \|V\|_p \leqslant M\} \tag{2.6}$$

(without loss of generality we could replace this with $S = \{\|V\|_p = M\}$), and assume $1 < p < \infty$. To spell out more of the argument sketched in Ref. 1, consider perturbations of the form

$$V_* \to V_* + \frac{\kappa\chi_{T_1}(x)}{\int_{T_1}|V_*|^{p-1}\,dx} - \frac{\kappa\chi_{T_2}(x)}{\int_{T_2}|V_*|^{p-1}\,dx},$$

where T_1 and T_2 lie in the interior of $\text{supp}(V_*)$, and where the coefficients of the characteristic functions χ_{T_1} and χ_{T_2} have been chosen so that the L^p norm of the perturbed potential equals M to first order in κ. Regular perturbation theory applies,[21] so if V_* is an optimizer for which the optimized eigenvalue is nondegenerate, and the eigenvalue associated with the perturbed potential is denoted $e(\kappa)$, then

$$0 = \frac{de}{d\kappa} = \frac{\int_{T_1}u_*^2\,dx}{\int_{T_1}|V_*|^{p-1}\,dx} - \frac{\int_{T_2}u_*^2\,dx}{\int_{T_2}|V_*|^{p-1}\,dx}$$

and leads to the conclusion that the derivative of the eigenvalue by κ can only be 0 for all admissible sets $T_{1,2}$ if the optimizing potential and its associated eigenfunction u_* are related algebraically via

$$u_*^2 = \text{const}\ |V_*|^{p-1}, \tag{2.7}$$

a.e. on $\text{supp}(V_*)$. Since this depends only on first-order perturbation theory, which states that the derivative of the eigenvalue is the expectation value of the perturbation in the unperturbed state, the argument of Ref. 1 still applies when $-\Delta$ is replaced by A or an even more general operator. It is also just as valid for minimizers as for maximizers, and is not sensitive to whether Ω is finite. More precisely stated: (2.7) is a necessary condition for any isolated, nondegenerate eigenvalue E_* to be either a maximum or a minimum over the set S. Unlike the case of predominant interest in Ref. 1, i.e., $p = 1$, the support of V_* is not a proper subset of Ω.

Proposition II.5: Let V_* be a maximizing or minimizing potential for an L^p constraint $(p > 1)$, with an associated eigenvalue that is nondegenerate, and let S be as in (2.6). Assume any one of the following: (a) $\nu \geqslant 1$, $p > 1$, and the eigenvalue is the ground state; or (b) $A + V_*$ has the unique continuation property.

Then the support of V_* contains all of Ω.

Remarks: Support is defined as for generalized functions, i.e., as the support of the measure $V_*\,dx$, not as for classical functions. Particular conditions guaranteeing the unique continuation property (b) are[30,31] (c) $\nu = 1$, V_*dx is a bounded measure; and (d) $\nu \geqslant 2$, $p > \nu/2$, and $A = -\Delta$.

Proof: The technique of proof resembles the technique used for (2.7). Suppose that the lemma is false, and let x lie outside the support of V_*. Let T denote a small ball centered at x. Since the support is closed, a sufficiently small T lies outside it. Consider the perturbation

$$V_* \to V_* + \kappa\chi_T, \tag{2.8}$$

and let u_* and $e(\kappa)$ denote the normalized eigenfunction for V_* and the eigenvalue of the perturbed potential, respectively. The formula of first-order perturbation theory then reads

$$e'(0) = (u_*, \chi_T u_*).$$

The norm of the perturbed potential in (2.8) is $M + O(\kappa^p) = M + o(\kappa)$, so a necessary condition for V_* to be an extremizer is that $e'(0) = 0$ for all sufficiently small T. This implies that $u_* = 0$ a.e. outside $\text{supp}(V_*)$. By hypothesis this is a set of positive measure, and thus there is a contradiction with either the positivity of the ground state (case a) or the unique continuation property. ■

When combined with (2.7), this proof also yields the following proposition.

Propositon II.6: Let V_* be a maximizing or minimizing

potential with an associated eigenvalue that is nondegenerate, and let S be as in (2.6), with $p>1$. Then (2.7), i.e.,

$$u_*^2 = \text{const}|V_*|^{p-1},$$

holds throughout Ω. Since (2.7) gives us a purely algebraic relationship between the optimizing potentials and their associated eigenfunctions, it can be substituted into the eigenvalue equation to yield a characterization of the optimizers. Note that since the eigenvalue equation is linear in u_*, its normalization can be chosen so that the constant in (2.7) is 1. Then we find that any optimizer (with a nondegenerate optimized eigenvalue) necessarily satisfies the generalization of Eq. (1.2),

$$Au \pm |u|^\alpha \operatorname{sgn}(u) = Eu, \tag{2.9}$$

where E is the associated eigenvalue, $\alpha = (p+1)/(p-1)$, and the equation has been written in terms of the associated eigenfunction, dropping the *. The upper sign obtains if the potential is a maximizer and the lower if it is a minimizer. An interesting consequence of the existence theory of maximizers is thus a proof of existence and certain properties of solutions of the necessary condition (2.9). The existence theory of (2.9), especially when $A = -\Delta$, the sign is negative, and $\alpha<(\nu+2)/(\nu-2)$, has been heavily studied; for instance, see Refs. 8, 9, 32, and 33. While the theory is already fairly well established, we wish to note that an alternative and rather painless analysis is possible in some cases as a consequence of our existence theorems for optimizers. The difference, in essence, is that while it is traditional to discuss (2.9) as the Euler equation for a functional, we choose a different functional, which has an L^2 setting, allowing more direct use of the spectral theorem. Let us restrict our attention to the ground state, which is automatically nondegenerate with a positive eigenfunction:

Corollary II.7: Let Ω be bounded and $\alpha>1$. For any $\Lambda>E(0)$ (= the fundamental eigenvalue of the operator A) and any $c>0$, the nonlinear eigenvalue problem

$$Au + cu^\alpha = \Lambda u \tag{2.10}$$

has a positive solution $u\in W_0^{1,2}(\Omega)$.

Remarks: (1) If the coefficients in A, W, and $\partial\Omega$ (supposing that Ω has a boundary) are smooth, and α is sufficiently small, then u will be smooth by elliptic regularity.

(2) This equation arises in the study of the relationship between Laplace–Beltrami operators and Schrödinger operators, and has recently been used to demonstrate the existence of Laplace–Beltrami operators on R^ν with periodic metrics and gaps in their spectra for $\nu>1$ (cf. Ref. 34).

Proof: We suppose $c=1$; this can always be achieved by scaling the function u. The existence of a potential V_* maximizing the ground-state eigenvalue of $A+V$ subject to $\|V\|_p = M$ for any $M>0$ is known from Theorem II.1, with $\alpha=(p+1)/(p-1)$. If the maximized eigenvalue is E_*, then the necessary condition (2.9) becomes (2.10) with $u=u_*$ and $\Lambda=E_*$. The theorem will thus be proved if it is shown that E_* increases continuously from $E(0)$ to ∞ as M goes from 0 to ∞. That it increases monotonically between these limits is obvious. Continuity follow from the fact that perturbations $\kappa P(x)$ with bounded functions $P(x)$ affect both the spectrum and the L^p norm continuously. [Strict monotony, needed below, follows similarly with positive, bounded $P(x)$.] ■

With the other sign we recover a variant of results described in Refs. 8, 9, and 32.

Corollary II.8: Suppose Ω is bounded and smooth, and $A=-\Delta+W$, with $W\in L^p$, $p>\nu/2$. Then for any $\Lambda<E(0)=\inf \text{sp}(A)$, and any $1<\alpha<\infty$ (if $\nu=1$ or 2) or $<(\nu+2)/(\nu-2)$ (if $\nu>2$), the nonlinear eigenvalue problem

$$Au - cu^\alpha = \Lambda U \tag{2.11}$$

has a positive solution in $W_0^{1,2}(\Omega)$ (which will be smooth if W is smooth).

The proof is just like the previous one, except that it relies on the existence of minimizers guaranteed by Corollary II.4. This corollary could be extended to guarantee the existence of certain other (not everywhere positive) solutions of (2.10) and (2.11) and of equations with other elliptic operators A.

III. OPTIMIZING POTENTIALS IN ONE DIMENSION

A. Preliminaries and general results

The general conclusions of Sec. II apply, of course, to the one-dimensional case, where, at least for Dirichlet or Neumann boundary conditions, the eigenvalues are automatically nondegenerate. The equation characterizing the optimizers (2.9) reduces to an ordinary differential equation, which can be interpreted as Newton's equation for an autonomous system. Following up on this idea, which was used by Glaser *et al.*[3] in the context of a very similar equation that also arose in the context of an optimization involving the Schrödinger equation, allows us to characterize the optimizing potentials rather explicitly. We call the independent variable t because of this interpretation. For definiteness, we take $A=-d^2/dt^2$ and $\alpha>1$ throughout this section, so that (2.9) becomes

$$\frac{d^2u}{dt^2} = \pm \operatorname{sgn}(u)|u|^\alpha - Eu. \tag{3.1}$$

Only three domains need be considered, a finite interval $[0,l]$, the semi-infinite interval $[0,\infty)$, and the line $\mathbb{R}=(-\infty,\infty)$. On the other hand, we wish to broaden our scope by considering a variety of self-adjoint boundary conditions in addition to those of Dirichlet type. The status of the existence question depends somewhat on whether the interval is finite or infinite and, if infinite, on what sort of boundary condition is imposed at the finite end point. We recall that if $\Omega=[0,\infty)$ or $(-\infty,\infty)$, then there is continuous spectrum $[0,\infty)$. If we define eigenvalues by the min–max principle, it may happen that $E_k(V)=0$ and fails to be a proper L^2 eigenvalue for finite k.

We shall only consider the self-adjoint boundary conditions

$$\begin{aligned} f'(0) &= mf(0), \\ f'(l) &= \pm mf(l), \quad m \text{ real} \end{aligned} \tag{3.2}$$

or Dirichlet conditions,

$$f(0)=0, \quad f(l)=0$$

[formally, $m=\infty$ in (3.2)].

Definition: When $\Omega = [0,l]$ or $[0,\infty)$, the index k of the eigenvalue $E_k(V)$ will always be taken as the number of nodes for $0 < t \in \Omega$. When $\Omega = (-\infty,\infty)$, k is the total number of nodes for $-\infty < t < \infty$.

This ordering, which is somewhat traditional for ordinary differential equations, corresponds to that of the min–max principle when $E_k(V)$ is an L^2 eigenvalue with the proper boundary conditions. It means, however, that on $[0,l]$ the Neumann eigenvalues ($m = 0$) are numbered

$$E_0 < E_1 < E_2 \cdots ,$$

whereas the Dirichlet eigenvalues are numbered

$$E_1 < E_2 < E_3 \cdots .$$

The m eigenvalues may follow either numbering, depending on the problem. Theorem III.2 shows that it is the right convention for our problem.

Theorem III.1: Suppose Ω is a finite, semi-infinite, or infinite interval with Dirichlet or m boundary conditions (3.2) imposed at any finite end points: For I a fixed finite interval which is possibly equal to $[0,l]$, and $p > 1$, let $S = \{f \in L^p \mid \|f\|_p \leqslant M, \operatorname{supp} f \subset I\}$. Let $E_k(V)$ denote the k th eigenvalue of $-d^2/dt^2 + V$. Then $E_k(V)$ attains its maximum and minimum on S (but might be trivially 0 if there is a continuum). If $\Omega = [0,l]$ or the optimum lies below the continuum, then the associated eigenfunction at optimization satisfies (3.1) on the interval I.

Proof: Existence has already been shown for bounded intervals, and the boundedness of the support is all that matters in that proof. The eigenvalues are automatically nondegenerate, so the characterizing equation (3.1) always applies. □

Except under some circumstances for the ground state, the maximizing problem degenerates into the continuum when Ω fails to be finite. On the other hand, it is an elementary min–max exercise with widely spaced square wells to see that there can be arbitrarily many negative eigenvalues no matter how small the L^p norm of the potential, so minimized eigenvalues are honestly eigenvalues if I is large enough. The question of the existence of minimizers on infinite intervals without the finite-support restriction is more involved. Because the operator $-d^2/dt^2 + V$ is defined with a core of compactly supported functions, one can consider first the minimizers on a finite interval and let the length of the interval tend to infinity. In essence, if the minimizers remain localized, then their limit is the minimizer for the infinite interval, but if they move to infinity, then the infinite interval has no minimizer. We shall see below that minimizers exist for the interval $\mathbb{R}$ or the interval $[0,\infty)$ with Neumann boundary conditions, but not for $[0,\infty)$ with Dirichlet boundary conditions. *If* minimizers exist, then they satisfy (3.1) with the negative sign.

Interpreting (3.1) as Newton's equation for a one-dimensional oscillator, we can identify what we call the classical potential energy as

$$W(u;E) = Eu^2/2 \mp |u|^{\alpha+1}/(\alpha+1) , \tag{3.3}$$

and the equation of conservation of classical energy is

$$u'^2/2 + W(u;E) = h , \tag{3.4}$$

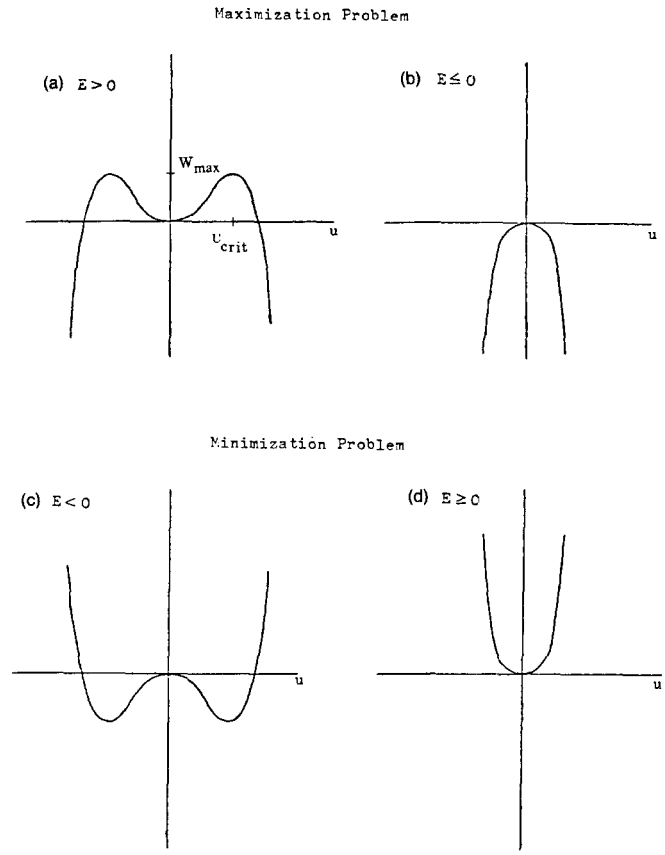

FIG. 1. Typical graphs of the classical potentials $W(u;E)$. Maximization problem: (a) $E > 0$, (b) $E \leqslant 0$; Minimization problem: (c) $E < 0$, (d) $E \geqslant 0$.

where we have used h to denote the parameter we shall refer to as the classical energy. See Fig. 1 for the graph of W. Note that the quantum energy E appears as a parameter in the classical potential energy, which can be viewed as a spring constant for the harmonic part of the potential when $E > 0$. The quantum potential appears only via u. The boundary conditions appear as an initial condition coupled with a final condition ($t = l$). Thus the Dirichlet and m boundary conditions (3.2) for $[0,l]$ with the $+$ sign, which we designate $+m$ boundary conditions, correspond to classical trajectories that execute $k/2$ closed orbits, k integral. (Phase diagrams are shown in Fig. 2.)

Remark: To determine the numbers E_k^* and optimizing potentials V_k^* one first solves (3.1), treating E as a parameter, for trajectories with the proper initial and final conditions and number of nodes, and then uses the algebraic condition (2.7) to determine $M = \|V\|_p$ from u by performing an integral. When several candidates for the optimizer occur the one giving the smallest value to M is selected. The inverse of the function thus defined gives E_k^* as a function of M. As noted in the proof of Corollary II.7, the optimal eigenvalue is strictly monotonic and continuous, so this is well defined. In addition, the set of allowed values of E_k for a given problem is exactly $[E_k(0),\infty)$ or $(-\infty,E_k(0)]$, as appropriate, where $E_k(0)$ is the k th eigenvalue of the potential $V \equiv 0$.

This point of view allows some general properties of the optimizers to be read off even without detailed analysis.

Proposition III.2: Consider the maximizing (resp. mini-

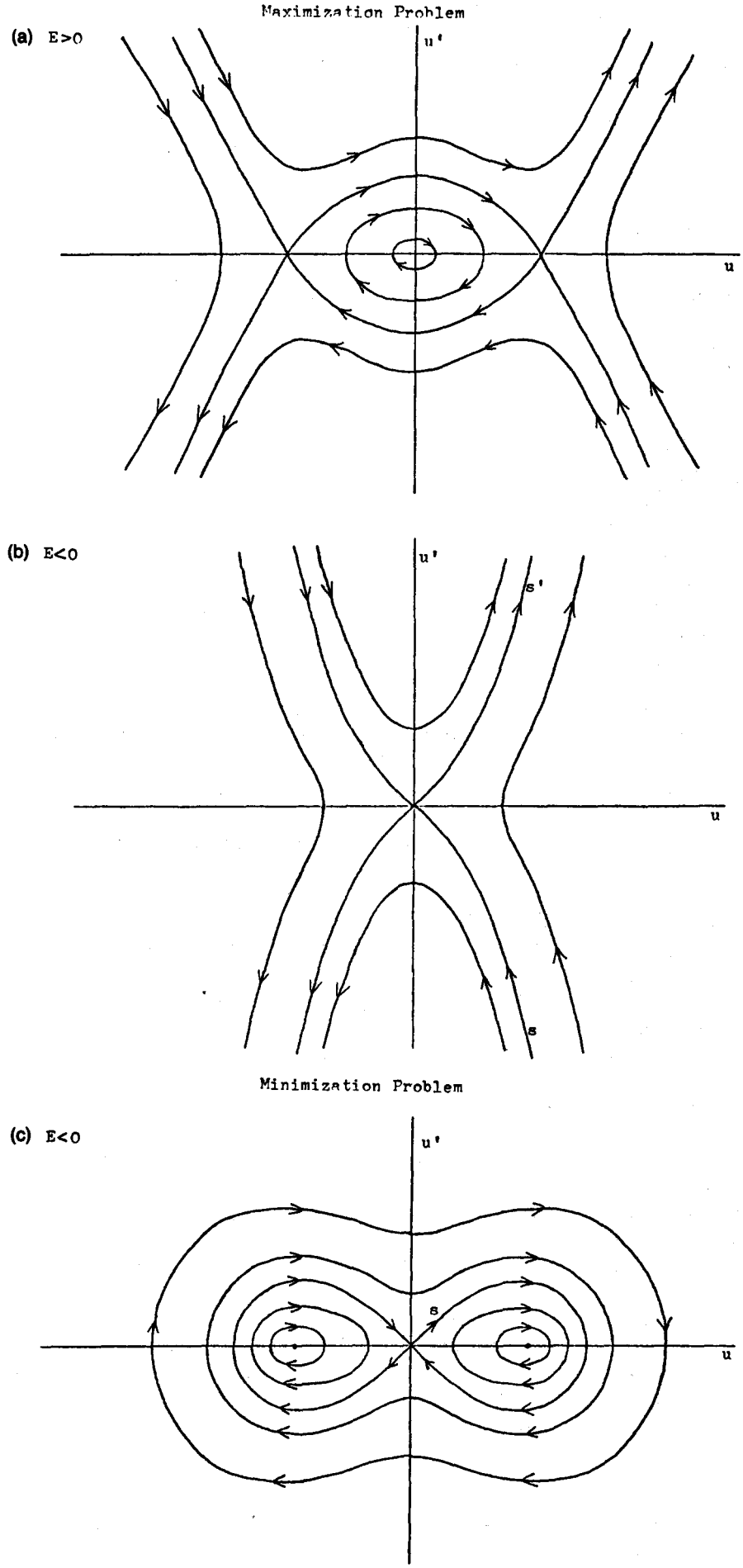

FIG. 2. Typical phase space portraits. Maximization problem: (a) $E>0$; (b) $E<0$; Minimization problem: (c) $E<0$,(d) $E>0$.

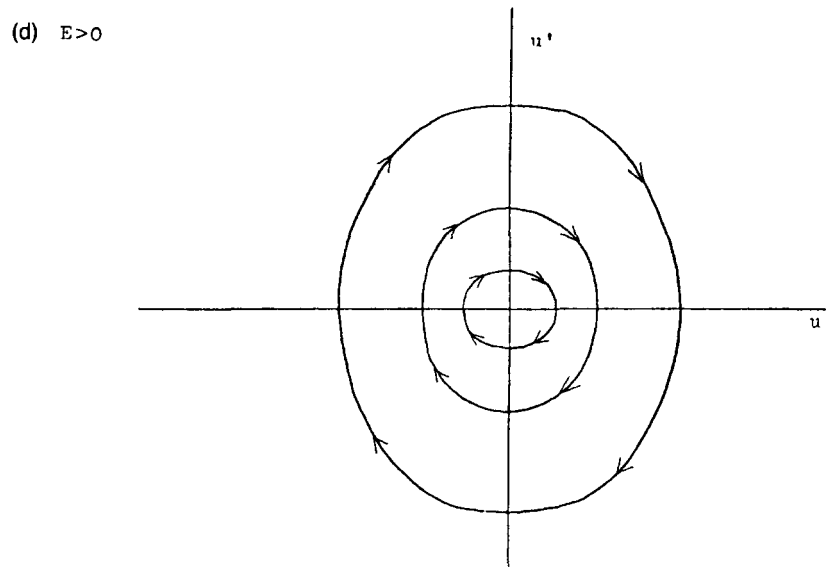

FIG. 2. (*Continued.*)

mizing) problem for any fixed $p>1$, M, $k>0$, and the finite interval. The maximized (minimized) eigenvalues are the same for the Dirichlet problem and all $+m$ boundary conditions. The maximizing (minimizing) potentials in these cases are periodic translates of the maximizer (minimizer) V_{*D} for the Dirichlet problem, which is smooth and positive except at its nodes and has the following symmetries for integers j, $0\leqslant j\leqslant k$:

$$V_{*D}(l-t)=V_{*D}(t)\,, \tag{3.5}$$

$$V_{*D}(jl/k)=0\,, \tag{3.6}$$

$$V_{*D}(t+jl/k)=V_{*D}(t)\,. \tag{3.7}$$

Proof: Because the eigenvalues are determined by the nodes, the determining equation (3.2) for all these cases corresponds to executing exactly $k/2$ closed orbits (cf. Fig. 2). The symmetry (3.5) reflects invariance under time reversal, since V is proportional to a power of $|u|$ by (2.7). Similarly, (3.6) and (3.7) just state that each orbit executed is identical, since the dynamical system is autonomous. Smoothness of u and the corresponding potential (away from zeros) arises from iterating the standard local smoothness theorems for solutions of the eigenvalue equation and applying (2.7). The integrals involving u that one has to perform have the same values for different boundary conditions, since they correspond to different starting points in the phase plane for the same number of identical half-orbits. Thus the functional relationships between the eigenvalue and M, whatever they are, are identical. □

Observe that the bottom Neumann eigenvalue is not covered, and in addition some m eigenvalues are excluded, because their eigenfunctions are nodeless (cf. Fig. 2). The dynamic geometry becomes more complicated for these anomalous trajectories enclosed in the separatrix, and will not be described here. Anomalous behavior occurs in the minimizing problem when $|m|<\sqrt{-E}$.

We note that one needs to deal with the case $E\leqslant 0$ in the maximization problem for the k th eigenvalue only if the boundary conditions are such that $H_0=-d^2/dt^2$ with these boundary conditions has its k th eigenvalue negative. Even then the maximal k th eigenvalue for a given M may well be positive (particularly if M is large). For Dirichlet and Neumann boundary conditions all eigenvalues of H_0 are non-negative so $E\leqslant 0$ need not be considered. The minimization problem on a finite interval will, however, require consideration of $E\geqslant 0$, particularly for higher eigenvalues, even for Dirichlet and Neumann boundary conditions. For minimization on an infinite or semi-infinite interval, on the other hand, one need only consider $E<0$.

From Eq. (3.1), one can derive certain useful integral identities relating

$$\int_\Omega \left(\frac{du}{dt}\right)^2 dt,\quad \int_\Omega u^2\,dt=\int_\Omega |V|^{p-1}\,dt\,,$$

and

$$\int_\Omega |u|^{\alpha+1}\,dt=\int_\Omega |V|u^2\,dt=\int_\Omega |V|^p\,dt\,.$$

If one multiplies through by u and integrates the derivative term by parts once one obtains

$$\int_\Omega \left(\frac{du}{dt}\right)^2 dt\pm\int_\Omega |u|^{\alpha+1}\,dt=E\int_\Omega u^2\,dt+\left(u\frac{du}{dt}\right)\Big|_{\partial\Omega}\,. \tag{3.8}$$

On the other hand, by integrating the conservation of the classical energy equation (3.4) over Ω, one finds

$$\frac{1}{2}\int_\Omega \left(\frac{du}{dt}\right)^2 dt\mp\frac{1}{\alpha+1}\int_\Omega |u|^{\alpha+1}\,dt+\frac{1}{2}E\int_\Omega u^2\,dt=h\,|\Omega|\,. \tag{3.9}$$

The two integral identities above, Eqs. (3.8) and (3.9), can be used to determine any two of $\int_\Omega u'^2\,dt$, $\int_\Omega u^2\,dt$, and $\int_\Omega |u|^{\alpha+1}\,dt$ in terms of the third. Note in this connection that since we scaled u to send the constant to 1 in the potential term of Eq. (3.1), we are *not* free to normalize u now. By

solving for $\int_\Omega u'^2 dt$ and $\int_\Omega |u|^{\alpha+1} dt$ in terms of $\int_\Omega u^2 dt$ we find

$$\|V\|_p^p = \int_\Omega |u|^{\alpha+1} dt$$

$$= \pm \frac{2p}{2p-1}\left[E\|u\|_2^2 - h|\Omega| + \frac{1}{2}uu'\Big|_{\partial\Omega}\right] \quad (3.10)$$

and

$$\|u'\|_2^2 = \frac{1}{2p-1}\left[-E\|u\|_2^2 + 2ph|\Omega| + (p-1)uu'|_{\partial\Omega}\right]. \quad (3.11)$$

B. Optimization for the line and the half-line

We are now ready to discuss the optimization problem for the line and half-line. In these cases the condition of square integrability of u at ∞ forces us to consider only those trajectories for which $u \to 0$ as $t \to \infty$ (and also $u \to 0$ as $t \to -\infty$ if $\Omega = \mathbf{R}$). This provides a further simplification since this can be accomplished only by trajectories of classical energy $h = 0$. Thus the energy relation simplifies to

$$\tfrac{1}{2}u'^2 + \tfrac{1}{2}Eu^2 \mp (\alpha+1)^{-1}|u|^{\alpha+1} = 0 \quad (3.12)$$

and the integral identity (3.10) becomes

$$\|V\|_p^p = \pm [2p/(2p-1)]\left[E\|u\|_2^2 + \tfrac{1}{2}uu'|_{\partial\Omega}\right]. \quad (3.13)$$

Equation (3.12) with the lower (+) sign has as its solutions

$$u(t) = (-pE/(p-1))^{(p-1)/2} \times \operatorname{sech}^{p-1}\left[\sqrt{-E}\,(t-c)/(p-1)\right], \quad (3.14)$$

where c is a constant of integration. The fact that we have a family of solutions which are all translates of one another reflects the fact that Eq. (3.12) is autonomous. The corresponding potential is given by

$$V(t) = [pE/(p-1)]\operatorname{sech}^2\left[\sqrt{-E}\,(t-c)/(p-1)\right], \quad (3.15)$$

which is familiar as the soliton solution to the Korteweg–de Vries equation when its variables are readjusted and interpreted appropriately. With the upper signs (maximization problem) these solutions are replaced by

$$u(t) = (-pE/(p-1))^{(p-1)/2} \times \operatorname{csch}^{p-1}\left[\sqrt{-E}\,(t-c)/(p-1)\right] \quad (3.16)$$

and

$$V(t) = [-pE/(p-1)]\operatorname{csch}^2\left[\sqrt{-E}\,(t-c)/(p-1)\right]. \quad (3.17)$$

For minimization on $\Omega = \mathbf{R}$, we find that for any choice of c in Eq. (3.15), $V(t)$ gives the same eigenvalues and has the same p norm. This is just a reflection of the fact that $\Omega = \mathbf{R}$ is translation invariant which leads to nonuniqueness of the minimizer for this problem. Computing $\|V\|_p^p$, we find

$$\|V\|_p^p = p^p(-E)^{(2p-1)/2}/(p-1)^{p-1}B(p,\tfrac{1}{2}), \quad (3.18)$$

where the beta function $B(p,\frac{1}{2})$ arises through use of the identity

$$\int_0^\infty \operatorname{sech}^\alpha x \tanh^\beta x\, dx = \frac{1}{2}B\left(\frac{\alpha}{2}, \frac{\beta+1}{2}\right).$$

We thus obtain the optimal lower bound in terms of $\|V\|_p$ for the ground state

$$E_0(V) \geq -[(p-1)^{p-1}/p^pB(p,\tfrac{1}{2})]^{2/(2p-1)}\|V\|_p^{2p/(2p-1)}. \quad (3.19)$$

This result was derived by Veling[13b] by quite different means. If one defines the optimal bound given on the right above as $h_{\mathbf{R}}(M)$ where $M = \|V\|_p$, that is,

$$h_{\mathbf{R}}(M) = -[(p-1)^{p-1}/p^pB(p,\tfrac{1}{2})]^{2/(2p-1)}M^{2p/(2p-1)}, \quad (3.20)$$

then the corresponding bounds on $\mathbf{R}^+$ with either Dirichlet or Neumann boundary conditions, denoted by $h_{\mathbf{R}^+,D}(M)$ and $h_{\mathbf{R}^+,N}(M)$, respectively, are given by

$$h_{\mathbf{R}^+,N}(M) = h_{\mathbf{R}}((2M^p)^{1/p}) = 2^{2/(2p-1)}h_{\mathbf{R}}(M) \quad (3.21)$$

and

$$h_{\mathbf{R}^+,D}(M) = h_{\mathbf{R}}(M). \quad (3.22)$$

These bounds were also first derived by Veling.[13a] By way of explaining these bounds from our perspective we note that the Neumann ground state on $\mathbf{R}^+$ corresponds to the ground state on $\mathbf{R}$ but that in passing from $\mathbf{R}^+$ to $\mathbf{R}$ via reflection we double M^p. Alternatively, we could observe that Neumann boundary conditions force $c = 0$ in Eq. (3.15). The situation for Dirichlet boundary conditions is somewhat more complicated. Here there is no optimizing potential but the $c \to \infty$ limit of Eq. (3.15) is seen to produce an approach to the optimal bound $h_{\mathbf{R}^+,D}(M)$. We therefore have the strict bound

$$E_0(V) > h_{\mathbf{R}^+,D}(M) \quad (3.23)$$

for the ground state energy of the Dirichlet problem on the half-line. Lack of an optimizing potential prevails in the cases where $\Omega = \mathbf{R}$ or $\mathbf{R}^+$ for all higher eigenvalues since there are no trajectories that cross the u axis in these cases.

Optimal bounds for higher eigenvalues will now be given. These bounds were not considered by Veling nor could they have been found by his methods. The heuristic argument given here will be justified only after we have analyzed the finite-interval problems since we will use a limiting argument to pass from these back to the infinite and semi-infinite interval problems. For a given value of M, our best strategy for minimizing $E_k(V)$ is to have $E_0(V),\ldots,E_k(V)$ be very close together by spreading V out into $k+1$ similar but widely separated wells. For an infinite or semi-infinite interval we can move these $k+1$ arbitrarily far apart and thereby make $E_i(V)$ for $i = 0,\ldots,k$ come arbitrarily near to each other and to the lowest eigenvalue that would be supported by any one of the wells individually. It is not cost effective with respect to our constraint M to use fewer (or more) than $k+1$ distinct wells in trying to minimize the $(k+1)$th eigenvalue. Indeed, a single well in one dimension may only support one eigenvalue while k widely spaced wells can be made to support k eigenvalues if the spacing is made sufficiently large. This reasoning suggests that for $\Omega = \mathbf{R}$ and for

$\Omega = \mathbb{R}^+$ with Dirichlet boundary conditions

$$E_k(V) > h_{\mathbb{R}}((\|V\|_p^p/(k+1))^{1/p}) = (k+1)^{-2/(2p-1)} h_{\mathbb{R}}(\|V\|_p) \text{ for } k \geqslant 1 \quad (3.24)$$

while for $\Omega = \mathbb{R}^+$ with Neumann boundary conditions

$$E_k(V) > h_{\mathbb{R}}((\|V\|_p^p/(k+\tfrac{1}{2}))^{1/p}) = (k+\tfrac{1}{2})^{-2/(2p-1)} h_{\mathbb{R}}(\|V\|_p) \text{ for } k \geqslant 1 . \quad (3.25)$$

These are optimal bounds for $E_k(V)$ in terms of $\|V\|_p$. The bounds for $\mathbb{R}^+$ with either Dirichlet or Neumann boundary conditions could also be obtained from that for $\mathbb{R}$ by exploiting the relation between E_{2k} for $\mathbb{R}$ and E_k for $\mathbb{R}^+$ with Neumann conditions and between E_{2k+1} for $\mathbb{R}$ and E_k for $\mathbb{R}^+$ with Dirichlet conditions. Note that there can be no bound in terms of $\|V\|_p$ to the number of negative eigenvalues in any of these problems. However, the results above lead rather effortlessly (in fact, are equivalent) to bounds on $N_E(V)$, the number of eigenvalues less than or equal to $E<0$. The bound on $N_E(V)$ arising in this way when $\Omega = \mathbb{R}$ is a special case of a result of Glaser, Grosse, and Martin [cf. Ref. 2, p. 203, Eq. (28) with $t=1$]. Their general result follows from the special result used in conjunction with the min–max principle; a particularly simple consequence is that $\|V\|_p$ may be replaced by $\|V_-\|_p$ in all our bounds [here $V_-(t) \equiv \min(0, V(t))$]. In addition, we remark that the bound on $N_E(V)$ of Ref. 2 also applies when $\Omega = \mathbb{R}^+$ with the Dirichlet boundary condition, whereas with the Neumann boundary condition an extra $\frac{1}{2}$ must be added to that bound.

We turn now to the case where $\Omega = \mathbb{R}^+$ with general boundary conditions of the form

$$u'(0) = mu(0), \quad m \in \mathbb{R}. \quad (3.26)$$

To see what E's would be reasonable candidates as eigenvalues for this problem we observe that $E_0(0) = 0$ if $m \geqslant 0$ and $E_0(0) = -m^2$ if $m<0$. Thus for the minimization problem any $E<0$ is a reasonable candidate for all E_k's if $m \geqslant 0$ and for all E_k's with $k \geqslant 1$ if $m<0$ but only E's less than $-m^2$ are reasonable candidates for E_0 if $m<0$.

Similarly, for the maximzation problem we need only consider E_0 for $m<0$ and then only E's in the range $-m^2 < E < 0$ are reasonable candidates as maximal eigenvalue. For the minimization problem, we can meet the boundary condition (3.26) if we choose c in Eq. (3.15) to satisfy

$$m = \sqrt{-E}\, \tanh(\sqrt{-E}\, c/(p-1)) . \quad (3.27)$$

Since the range of tanh is $(-1,1)$ and tanh is strictly increasing, this equation will have a unique solution c if and only if $|m| < \sqrt{-E}$ or, equivalently, $E < -m^2$. Thus for fixed m there will be a ground state minimizing potential associated with each $E < -m^2$, whereas for $0 > E \geqslant -m^2$ there will not be. However, when $m>0$ and $0 > E \geqslant -m^2$ we will be able to construct sequences of approximate minimizers (a minimizing sequence of potentials) and thereby determine optimal bounds on the eigenvalue as was done above for the Dirichlet problem. Such considerations also apply to higher eigenvalues as before. The optimal lower bound for the lowest eigenvalue is now given implicitly by the relations

$$\|V\|_p^p = \frac{p^p(-E)^{(2p-1)/2}}{2(p-1)^{p-1}} \times \left[B\left(\frac{1}{2}, p\right) + (\operatorname{sgn} m) B\left(\frac{-m^2}{E}; \frac{1}{2}, p\right)\right] \quad (3.28)$$

for $E < -m^2$, where the incomplete beta function, $B(x;p,q)$, is defined by

$$B(x;p,q) = \int_0^x t^{p-1}(1-t)^{q-1}\, dt \text{ for } 0 \leqslant x \leqslant 1 . \quad (3.29)$$

For all $m \geqslant \sqrt{-E}$ the Dirichlet optimal bound, Eq. (3.22), applies. For fixed E, it is of interest to see how classical oscillator trajectories come into play with reference to Fig. 2(c). Actually, only the trajectory labeled s (for separatrix) is needed in this analysis. Our parameter m governs the slope of the line whose intersection with this trajectory is our initial position. For $-\sqrt{-E} < m < \sqrt{-E}$ a segment of trajectory is cut off and this segment determines the optimizing potential and wave function that go with our chosen value of E. As m increases across this interval we include more and more of the trajectory until at $m = \sqrt{-E}$ the whole trajectory is included. This corresponds to c, the position of the center of the sech^2 well, moving from $-\infty$ to ∞. As m moves on up from $\sqrt{-E}$, m has no further effect on the optimal relation between $E_0(V)$ and $\|V\|_p$. On the other hand, as m moves on down from $-\sqrt{-E}$, one finds that the eigenvalue $E_0(0) = -m^2$ of the same problem with no potential is less than E and so E can never be a minimal lowest eigenvalue for these problems. Higher eigenvalues can be treated analogously. In place of Eq. (3.28), one obtains

$$\|V\|_p^p = \frac{p^p(-E_k)^{(2p-1)/2}}{2(p-1)^{p-1}} \times \left[(2k+1) B\left(\frac{1}{2}, p\right) + (\operatorname{sgn} m) B\left(\frac{-m^2}{E_k}; \frac{1}{2}, p\right)\right] \quad (3.30)$$

for $E < -m^2$; for $m \geqslant \sqrt{-E}$ one obtains the Dirichlet answer, Eq. (3.24), and for $m \leqslant -\sqrt{-E}$ one obtains the Dirichlet answer with index adjusted by 1. Lastly, we consider briefly the maximization problem for the ground state when $m<0$. We need only concern ourselves with the case of $m < -\sqrt{-E}$. From Eqs. (3.16) and (3.26), the relation between the parameters m and c is found to be

$$m = \sqrt{-E}\, \coth[\sqrt{-E}\, c/(p-1)] . \quad (3.31)$$

Also the optimal relation between $E_0(V)$ and $\|V\|_p$ is given by

$$\|V\|_p^p = [p^p(-E)^{(2p-1)/2}/2(p-1)^{p-1}] \times B(1 + E/m^2;\ p,\ \tfrac{1}{2} - p) , \quad (3.32)$$

where $-m^2 < E < 0$. Note that the beta function ranges from 0 to ∞ as m ranges from $\sqrt{-E}$ to $-\infty$ since the argument $\frac{1}{2} - p$ makes $B(x;p,\frac{1}{2}-p)$ singular as $x \to 1^-$. This is in accord with the qualitative phase space analysis [see Fig. 2(b)] where we cut off various parts of trajectory s for

$-\infty < m < -\sqrt{-E}$, including more and more of the diverging part as $m \to -\infty$.

C. Optimization for finite intervals

For finite interval problems we can no longer confine our attention strictly to trajectories of classical energy $h = 0$. Since we shall deal primarily with Dirichlet and Newmann boundary conditions and their associated family of equivalent boundary conditions (see Proposition III.2) it is useful to begin with a treatment of the periods of the classical orbits which occur in the various cases. In the maximization problem with $E > 0$, one finds that the classical period $T(h,E)$ ranges monotonically from the harmonic oscillator limit, $2\pi/\sqrt{E}$, as $h \to 0^+$ to ∞ as h approaches the maximum value of the classical potential. This can be seen from the expression

$$T(h,E) = 4\int_0^{u_1} \frac{du}{\sqrt{2}(h - W(u;E))}, \tag{3.33}$$

where u_1 is the first positive turning point of the classical motion. A detailed analysis of the period function T in a general setting is to be found in Refs. 35–37. By changing variables to $s = u/u_1$ and writing h in terms of u_1 via $h = W(u_1;E)$ we obtain

$$T(h,E) = 4\int_0^1 \frac{ds}{\sqrt{E}\,(1-s^2) - [2/(\alpha+1)]u_1^{\alpha-1}(1-s^{\alpha+1})}. \tag{3.34}$$

Now as is evident from Fig. 1(a), u_1 is a strictly increasing function of h for the range of h's we are considering and hence we may analyze how T changes as h varies from 0 to the maximum value of the classical potential by seeing how expression (3.34) changes as u_1 increases from 0 to the position of the maximum of the classical potential. Since the integrand increases with u_1 for all $s \in [0,1)$, it is clear that T is strictly increasing as a function of u_1 and hence also as a function of h. For the minimization problem with $E < 0$ the classical orbits fall into two classes: those with $h > 0$ and those with $h < 0$. By an analysis almost identical to that given above we arrive at

$$T(h,E) = 4\int_0^1 \frac{ds}{\sqrt{[2/(\alpha+1)]u_1^{\alpha-1}(1-s^{\alpha+1}) + E(1-s^2)}} \tag{3.35}$$

for the case where $h > 0$. This time h ranging from 0 to ∞ corresponds to u_1 increasing monotonically from $u_{1,\min}$ [defined by $W(u_{1,\min};E) = 0$, $u_{1,\min} > 0$] to ∞ which in turn corresponds to T decreasing from ∞ to 0. Next we consider the orbits having $h < 0$. The result is much like that for Fig. 1(a) in that T is found to approach a harmonic oscillator limit, $2\pi/\sqrt{(\alpha-1)(-E)}$, as h approaches the minimum value of the classical potential and to increase to ∞ as h increases to 0. $T(h;E)$ is continuous and positive for h in the range described. The question of whether or not it is monotonic is difficult. Recent results of Chicone[38] and of Chow and Wang[39] can be used to show that T is monotone increasing in h for $h < 0$ and for all $p > 1$. Later in this paper we shall explicitly treat the case where $p = 2$ in terms of elliptic functions as a preliminary to settling further questions for this case. Lastly we consider the case arising from the minimization problem with $E \geqslant 0$ [Fig. 2(d)]. When $E > 0$ it is easy to show that T ranges monotonically from the harmonic oscillator limit, $2\pi/\sqrt{E}$, down to 0 as h varies from 0 to ∞. When $E = 0$, T ranges monotonically from ∞ to 0 for the same variation of h.

The considerations above are of use to us for the Dirichlet and Neumann optimization problems on a finite interval $[0,l]$ through the following observations: for the function $u(t)$ associated with an optimizer of E_k to meet Dirichlet or Neumann boundary conditions it must execute an integral number of half-orbits in time l. The integer occurring here is associated with the index k; in fact, for the Dirichlet and Neumann problems we have the condition

$$kT(h,E_k)/2 = l \quad \text{for } k = 1,2,3,..., \tag{3.36}$$

though for $k = 0$ in the Neumann minimization problem we have the condition

$$(j/2)T(h,E_0) = l \quad \text{for some } j \in \{1,2,3,...\}. \tag{3.37}$$

Also critical points on the u axis will have to be examined in the Neumann problems. We remark that these conditions are to be viewed as conditions determining values of h which are allowed by some given choice of E and k. If for such a choice we have several classical orbits or critical points which give candidates for optimizers we will have to decide among these by computing the values of $\|V\|_p$ associated with them and taking the candidate which gives the least value. To the extent that the conditions above lead to a single candidate we will have characterized the unique optimizer. For the sake of reference we list the eigenvalues of $-d^2/dt^2$ with $+m$ boundary conditions. They are

$$E_k(0) = (k\pi/l)^2, \quad k = 1,2,3,... \tag{3.38}$$

and

$$E_0(0) = -m^2 \tag{3.39}$$

with the latter eigenvalue present for all $m \in \mathbb{R}$ (but not for Dirichlet boundary conditions, which correspond to $m \to \pm\infty$).

Let us now give brief discussions of each of the most standard finite interval cases individually. For the Dirichlet maximization problem our discussion of periods allows us to find exactly one maximizing candidate for any choice of E and k so long as $2l/k > 2\pi/\sqrt{E}$. Thus if

$$E > (k\pi/l)^2 = E_k(0) \quad \text{for } k \in \{1,2,3,...\}, \tag{3.40}$$

E will arise as a maximal value $E_k^*(M)$ for some choice of $M > 0$ and we have an explicit characterization of the maximizing potential and eigenfunction. This same analysis applies to the higher eigenvalues ($k \geqslant 1$) for the Neumann maximization problem. For the ground state the only candidate for the maximizer comes from the critical points not at the origin and we are done. Here E should be chosen to be positive. Theorem III.2 also allows the results above to be applied to the $+m$ boundary conditions, Eq. (3.2) with the

plus signs, which are related to Dirichlet and Neumann problems. With $+m$ boundary conditions the allowed values of E for ground state maximization are given by $E > -m^2$. When $E \leqslant 0$, this condition can be rewritten as $|m| > \sqrt{-E}$ and the trajectories that arise as candidates for yielding the maximizing potential are then found to be portions of phase curves in Fig. 2(b) lying above the curve s' or below the curve s, i.e., curves having positive classical energy h. When $E > 0$, one can find analogous nodeless solutions corresponding to trajectories having classical energy $h > W_{\max}$ [see Figs. 1(a) and 2(a)].

The Dirichlet minimization problem is almost as simple as the above since orbits with $h \leqslant 0$ are ruled out by the condition $u(0) = 0 = u(l)$. Allowed minimal E_k's are given by

$$E < E_k(0) = (k\pi/l)^2 \quad \text{for } k = 1,2,3,\ldots . \tag{3.41}$$

This condition could also be read off from our knowledge of the classical periods since for $E \leqslant 0$, T ranges between 0 and ∞ for $h \in (0,\infty)$ and for $E > 0$ T ranges from $2\pi/\sqrt{E}$ down to 0 so that only those E's for which $k\pi/\sqrt{E} > l$ or $E < (k\pi/l)^2$ are attainable as minimal E_k's for $M > 0$. When one considers the corresponding Neumann problem all the trajectories just discussed come back into play though not yet as unique minimizers since one now must contend with the additional orbits which occur when $h < 0$ and $E < 0$. First, we note that the constraint on choices for E_k, Eq. (3.41), still holds but now for $k = 0,1,2,\ldots$. Second, note that the situation for $E \geqslant 0$ is the same as before and thus we have already characterized the unique minimizing potentials for this case. When $E < 0$, however, we may now have two or more choices of orbits to consider as well as the critical points not at the origin. These may be sorted by node counting: note that the orbits or critical points for which $h < 0$ have no nodes [see Fig. 2(c)] and hence can at most be candidates as minimizers of the ground state. At this point higher states are all uniquely characterized but there remains the question of whether the ground state minimizer comes from the critical point (implying a constant potential) or from an $h < 0$ orbit. Each $h < 0$ orbit leads to two optimizing candidates corresponding to the two possible starting points. Since both choices lead to the same M value, if such an orbit gives rise to a minimizer it gives rise to a second minimizer as well and we would therefore have a nonunique minimizer. The situation for $+m$ boundary conditions is even somewhat more involved. Again, by the node-counting argument the $h < 0$ orbits are only of importance when looking for the ground-state minimizer.

Furthermore, one can show that the classical Hamiltonian function, $h(u,u')$, is an increasing function of radial distance from the origin $(u,u') = (0,0)$ on the region of the phase plane outside the separatrix s, which is the figure-eight-shaped curve formed by the $h = 0$ trajectories [see Fig. 2(c)]. Thus any ray from the origin intersects each $h > 0$ orbit exactly once and, in addition, we need only consider the $h < 0$ orbits when m and our choice of E are related by $|m| < \sqrt{-E}$. This last condition comes from the fact that the $h = 0$ trajectories enter the origin with asymptotic slope $\pm\sqrt{-E}$. When $|m| < \sqrt{-E}$ there will surely be a nodeless solution and thus E can be an E_0^* as in the Neumann case.

D. Bounds on the number of negative eigenvalues for finite-interval problems

We turn now to the topic of finding bounds in terms of $\|V\|_p$ on the number $n(V)$ of negative eigenvalues for the operator $H_V = -d^2/dt^2 + V(t)$ acting on $L^2(0,l)$ with Dirichlet or, more generally, $+m$ boundary conditions. This problem is especially tractable since we need only deal with the $E = 0$ case of the minimization problem. This eliminates a term from Eq. (3.4) and allows us to solve explicitly for the period

$$T(h,0) = 2\sqrt{2}h^{-1/2p}((p-1)/2p)^{(p+1)/2p}B((p-1)/2p,\tfrac{1}{2}); \tag{3.42}$$

in addition, the integral identity (3.10) reduces to

$$\|V\|_p^p = [2p/(2p-1)]hl . \tag{3.43}$$

Thus in the case of Dirichlet boundary conditions, for V to admit the possibility of having k negative eigenvalues we must have

$$\|V\|_p^p > [k^{2p}(p-1)^{p+1}/(2p-1)l^{2p-1}p^p] \times B((p-1)/2p,\tfrac{1}{2})^{2p} \tag{3.44}$$

and, since $+m$ boundary conditions simply require an index shift, we have proved the following theorem.

Theorem III.3: The number of negative eigenvalues $n(V)$ of the operator $H_V = -d^2/dt^2 + V(t)$ acting on $L^2(0,l)$ subject to $+m$ boundary conditions and with $V \in L^p(0,l)$, $1 < p < \infty$, $V_- \not\equiv 0$, satisfies the bound

$$n(V) < 1 + \frac{p^{1/2}\|V_-\|_p^{1/2}}{B((p-1)/2p,\tfrac{1}{2})}\left[\frac{(2p-1)l^{2p-1}}{(p-1)^{p+1}}\right]^{1/2p} . \tag{3.45}$$

In particular, (3.45) applies in the case of Neumann boundary conditions. The same bound applies in the case of Dirichlet boundary conditions if the additive 1 is deleted, and, furthermore, these bounds are optimal bounds for $n(V)$ in terms of $\|V_-\|_p$.

Remark: The part of this theorem dealing with Dirichlet boundary conditions was first proved by Grosse (cf. Ref. 40, p. 94, Proposition 1).

E. The Neumann ground state minimizer for $p=2$: A bifurcation phenomenon

Other problems which may be integrated in terms of the more standard special functions are the cases of Eq. (3.4) with $p = 2$ or 3 [corresponding to $\alpha = 3$ or 2, respectively, via $\alpha = (p+1)/(p-1)$] and general E. The solution $u(t)$ may then be expressed in terms of elliptic functions. Here we shall pursue the special case $p = 2$ with $E < 0$ in an effort to understand the ground state of the Neumann minimization problem which we left incompletely characterized in the case of general p.

Thus we must look at solutions to

$$u'^2 = 2h - Eu^2 - u^4/2 , \tag{3.46}$$

where $h < 0$ for which $u'(0) = 0 = u'(l)$. The critical point at $(u,u') = (\sqrt{-E},0)$ certainly yields one solution

$$u_0(t) = \sqrt{-E} . \tag{3.47}$$

To see what other solutions need to be considered, we observe that the general solution to Eq. (3.46) above is

$$u(t) = a\,\mathrm{dn}(at/\sqrt{2} - c, \mu)\,, \tag{3.48}$$

where dn represents one of the standard Jacobian elliptic functions.[41] Here c is the arbitrary constant of integration,

$$a = \sqrt{-E + (E^2 + 4h)^{1/2}} \tag{3.49}$$

and the parameter μ (= mod squared) of the elliptic function is given by

$$\mu = 1 - b^2/a^2\,, \tag{3.50}$$

where

$$b^2 = -E - \sqrt{E^2 + 4h}\,. \tag{3.51}$$

The constants a^2 and b^2 are simply the roots of the right-hand side of Eq. (3.46), when this is viewed as a quadratic in u^2. Now the period of $\mathrm{dn}(\cdot;\mu)$ is $2K(\mu)$, where $K(\mu)$ represents the complete elliptic integral of the first kind.[41] To meet the boundary conditions we impose

$$c = 0 \quad \text{or} \quad c = K(\mu) \tag{3.52}$$

and

$$l = jT(h;E)/2 = j(\sqrt{2}/a)K(\mu)\,, \quad \text{where} \quad j \in \{1,2,3,\ldots\}\,. \tag{3.53}$$

Before we can proceed, we must analyze the function $K(\mu)/a$ as a function of h for $-E^2/4 < h < 0$ [$-E^2/4$ is the minimum value of $W(u;E)$]. We will see that as h increases across this range $(\sqrt{2}/a)K(\mu)$ increases from the limiting value $\pi/\sqrt{-2E}$ to infinity. This may be shown as follows. First, we observe that μ and h are related by

$$\mu = 1 - (b^2/a^2) = 2\sqrt{E^2 + 4h}\,/(-E + \sqrt{E^2 + 4h}\,) \tag{3.54}$$

so that

$$\sqrt{E^2 + 4h} = \mu(-E)/(2 - \mu) \tag{3.55}$$

and thus

$$a^2 = 2(-E)/(2 - \mu)\,. \tag{3.56}$$

Now it is easy to show using calculus that μ increases monotonically from 0 to 1 as h increases from $-E^2/4$ to 0. Hence we will be done if we can show that

$$[(\sqrt{2} - \mu)/\sqrt{-E}\,]K(\mu) \tag{3.57}$$

is an increasing function of μ for $0 \leqslant \mu < 1$. To *verify* this we show that this expression has a positive derivative and this amounts to showing that

$$2(2 - \mu)\frac{dK}{d\mu}(\mu) > K(\mu) \quad \text{for } 0 < \mu < 1\,. \tag{3.58}$$

This inequality follows by demonstrating that the power series for $K(\mu)$ at $\mu = 0$, which has positive coefficients and radius of convergence 1, is majorized by that for $2(2 - \mu)dK/d\mu(\mu)$. Finally, it is easy to see that the limiting values are as stated above. This analysis shows that solutions (3.48) satisfying condition (3.53) do arise if

$$l > j\pi/\sqrt{-2E} \quad \text{for } j \in \{1,2,3,\ldots\}\,,$$

i.e., if

$$E < -\tfrac{1}{2}(j\pi/l)^2 \quad \text{for } j \in \{1,2,3,\ldots\}\,. \tag{3.59}$$

Therefore, we have the following situation: if $0 > E \geqslant -\pi^2/2l^2$ only the constant solution $u_0(t)$ is a minimizing candidate and hence it yields the minimizer, if $-\pi^2/2l^2 > E \geqslant -2\pi^2/l^2$ we have the constant solution plus two "$j = 1$ solutions" [coming from the two choices for c, Eq. (3.52)] as minimizing candidates, if $-2\pi^2/l^2 > E \geqslant 9\pi^2/2l^2$ we have the constant solution, two $j = 1$ solutions, and two $j = 2$ solutions as minimizing candidates, etc. Here we shall concentrate only upon what happens as E is decreased beyond the first critical value at $-\pi^2/2l^2$. This problem exhibits an interesting bifurcation.

Proposition III.4: The ground state minimizer for the Neumann problem on a finite interval of length l with $p = 2$ undergoes a bifurcation at $M^2 = \pi^4/4l^3$. For $0 < M^2 \leqslant \pi^4/4l^3$ the minimizing potential is a constant function, but for $M^2 > \pi^4/4l^3$ it is a (nonconstant) Jacobian elliptic function and is not unique.

Proof: For E between $-\pi^2/2l^2$ and $-2\pi^2/l^2$ the other solutions that we must consider are

$$u_{1a}(t) = a\,\mathrm{dn}(at/\sqrt{2}, \mu) \tag{3.60}$$

and

$$u_{1b}(t) = a\,\mathrm{dn}(at/\sqrt{2} - K(\mu), \mu) = a\,\mathrm{dn}(a(t - l)/\sqrt{2}, \mu)\,. \tag{3.61}$$

Since these solutions are simply reflections of each other in the line $t = l/2$ and since all associated p norms will therefore be identical we shall use only the subscript 1 (without the distinguishing a or b) for the most part. In the above, $K(\mu)$ and l are related by Eq. (3.53) with $j = 1$; we shall view this as an equation determining μ as a function of E (l is assumed fixed). So as to work with explicitly small parameters as an aid in identifying orders of small terms we introduce the scaled quantities ϵ and η via

$$E = (-\pi^2/2l^2)(1 + \epsilon)^2 \tag{3.62}$$

and

$$\mu = 2\eta\,. \tag{3.63}$$

The question of which of u_0 or u_1 provides the minimizer will be decided by a comparison of the norms $M_0 = \|V_0\|_2$ and $M_1 = \|V_1\|_2$. The solution yielding the smaller value of M will be the minimizer. We begin by determining the first few terms of the series for η in powers of $\epsilon^{1/2}$. This series is guaranteed to exist and have a nonzero radius of convergence by the analytic inverse function theorem applied to the function

$$F(z) = [(2/\pi)(1 - z)^{1/2}K(2z) - 1]^{1/2}\,. \tag{3.64}$$

This function is analytic at $z = 0$ and satisfies $F(0) = 0$, $F'(0) = \sqrt{3}/4$. Relation (3.53) with $j = 1$ can now be represented as just $\epsilon^{1/2} = F(\eta)$ if we substitute for a, E, and μ using Eqs. (3.56), (3.62), and (3.63). Solving for η as a series in $\epsilon^{1/2}$ one finds

$$\eta = (4/\sqrt{3})\epsilon^{1/2} - \tfrac{16}{3}\epsilon + (31/2\sqrt{3})\epsilon^{3/2} - \tfrac{116}{9}\epsilon^2 + \cdots \tag{3.65}$$

and solving in turn for h one obtains

$$h = (\pi^4/16l^4)\left[-1 + \tfrac{4}{3}\epsilon - \tfrac{2}{9}\epsilon^2 + O(\epsilon^3) \right] . \tag{3.66}$$

We can now proceed with the comparison of norms. Using the integral identity (3.10) we have (in self-explanatory notation)

$$\begin{aligned} M_1^2 - M_0^2 &= \tfrac{4}{3}\left[(-E)(\|u_1\|_2^2 - \|u_0\|_2^2) + l(h_1 - h_0) \right] \\ &= \frac{4}{3}\left[(-E)a\sqrt{2}\int_0^{K(\mu)} dn^2(s,\mu)ds + l(-E^2 + h_1 - h_0) \right] \\ &= \tfrac{4}{3}\left[(-E)a\sqrt{2}E(\mu) + \sqrt{2}K(\mu)\{E^2 + \tfrac{1}{4}\mu^2E^2/(2-\mu)^2\}/a \right] \\ &= \left[\sqrt{2}(-E)^{3/2}/3(1-\eta)^{3/2}\right]\left[4(1-\eta)E(2\eta) - (4 - 8\eta + 3\eta^2)K(2\eta)\right] , \end{aligned} \tag{3.67}$$

where $E(\mu)$ represents the complete elliptic integral of the second kind[41]; to avoid confusion with the energy E we shall always include the argument when writing this function. Now an easy computation shows that

$$\begin{aligned} &4(1-\eta)E(2\eta) - (4 - 8\eta + 3\eta^2)K(2\eta) \\ &\quad = -3\sum_{n=4}^{\infty} \frac{(n-2)(n-3)}{n(n-1)} \\ &\qquad \times \left[\frac{(2n-5)!!}{(2n-4)!!}\right]^2 2^{n-2}\eta^n \end{aligned} \tag{3.68}$$

and hence that $M_1^2 < M_0^2$ for all $0 < \eta < 1$. Thus the solutions u_{1a} and u_{1b} yield a lower ground state eigenvalue than u_0 for any $M^2 > \pi^4/4l^3$. Furthermore, at least for M^2 in the interval $\pi^4/4l^3 < M^2 \leqslant 4\pi^4/l^3$, these $j = 1$ solutions yield the minimizing potential since higher j solutions need not be considered. □

We note that after the bifurcation at $M^2 = \pi^4/4l^3$ ($E^* = \pi^2/2l^2$) the minimizing potential ceases to be symmetric under $t \to l - t$ (symmetry with respect to $t = l/2$) but rather we get two minimizing potentials which transform into each other under this operation. Since the problem as stated also shares this symmetry we may say that the symmetry of the ground state minimizer breaks at $M^2 = \pi^4/4l^3$ leading to nonuniqueness of the minimizer in this case. It is perhaps worthy to note that the nonuniqueness of the ground state minimizer for $\Omega = \mathbb{R}$ can be described in analogous terms: the original problem has translational symmetry and all the nonunique ground state minimizers transform into one another under translation. In addition, we conjecture that the $j = 1$ solutions give the minimizer for all $M^2 > \pi^4/4l^3$.

F. The case of "compact-support" boundary conditions

We next take up a discussion of what we call compact-support boundary conditions. In this category we consider the operator H_V on $L^2(\mathbb{R})$ or $L^2(\mathbb{R}^+)$, where $V \in L^p$ and V is further restricted to having its support in $[-l,l]$ or $[0,l]$. Here we shall focus our attention on the compact-support minimization problem on $\mathbb{R}$; optimization problems on $\mathbb{R}^+$ with various boundary conditions at $t = 0$ could be handled similarly. For this problem the compact-support condition implies that

$$u(t) = A_{\pm} e^{\mp\sqrt{-E}\,t} \quad \text{for} \quad \pm t \geqslant l , \tag{3.69}$$

where A_+ and A_- are arbitrary constants. These conditions lend themselves to viewing the problem as a problem on $[-l,l]$ with boundary conditions

$$u'(\pm l) = \mp\sqrt{-E}\,u(\pm l) , \tag{3.70}$$

which are what we call compact-support boundary conditions. Just as in all previous finite-interval problems we must first analyze the function giving the traversal times of our classical trajectories, that is, the times which our classical trajectories take in passing between the lines determined by the boundary conditions. Since our point of departure in these discussions is to fix E, that E appears in the boundary conditions is not an obstacle, in fact, in a certain respect it simplifies the calculation. (In this regard, it may be recalled that in our work with $+m$ boundary conditions the values $m = \pm\sqrt{-E}$ were found to be critical values at which the type of behavior encountered undergoes a transition.) We begin by looking at the traversal time for the ground state

$$T_c(h;E) = 2\int_{u_0}^{u_1} \frac{du}{\sqrt{2}(h - \tfrac{1}{2}Eu^2 - [1/(\alpha+1)]u^{\alpha+1})} . \tag{3.71}$$

Here u_1 is the positive turning point of the classical oscillator and $u_0 > 0$ gives its starting position: we start at the point $(u,u') = (u_0, \sqrt{-E}\,u_0)$ in phase space with classical energy $h = [1/(\alpha+1)]u_0^{\alpha+1} > 0$. We wish to see how $T_c(h;E)$ varies as h varies from 0 to ∞. First, it is clear that $T_c(h;E) \to \infty$ as $h \to 0^+$. Beyond this, we shall show that $T_c(h;E)$ decreases monotonically to 0 as h increases from 0 to ∞. To see this, we change variables in the by now familiar fashion, arriving at

$$\begin{aligned} T_c(h;E) = 2\int_{u_0/u_1}^{1} &ds/([2/(\alpha+1)]u_1^{\alpha-1}(1 - s^{\alpha+1}) \\ &+ E(1-s^2))^{1/2} . \end{aligned} \tag{3.72}$$

Now as h increases, u_1 increases so that the integrand decreases and we will be done if we can show that u_0/u_1 increases with h. This follows from the relation

$$[1/(\alpha+1)]u_0^{\alpha+1} = \tfrac{1}{2}Eu_1^2 + [1/(\alpha+1)]u_1^{\alpha+1} \tag{3.73}$$

rewritten as

$$u_0/u_1 = [1 - [(\alpha+1)/2](-E)u_1^{-(\alpha-1)}]^{1/(\alpha+1)}. \tag{3.74}$$

It also easily follows from this argument that $T_c(h;E) \to 0$ as $h \to \infty$. Since existence of a minimizer is established (Theorem III.1), we have the following proposition.

Proposition III.5: For any $p > 1$, k, l, and M, there is a unique potential satisfying $\|V\|_p \leqslant M$ and $\text{supp}(V) \subset [-l,l]$ which minimizes $E_k(V)$, the k th eigenvalue of $H_V = -d^2/dt^2 + V(t)$ acting on $L^2(\mathbb{R})$.

To be a bit more explicit, given an E and an l the ground state minimizer is provided by the classical trajectory whose classical energy h is determined by

$$2l = T_c(h;E). \tag{3.75}$$

We may proceed on to higher eigenvalues by observing that the required classical trajectories must be determined by the condition

$$2l = T_c(h;E) + kT(h;E)/2, \tag{3.76}$$

where $T(h;E)$ is the function giving the period of the associated closed orbit considered previously [Eq. (3.35)] and $k \in \{1,2,3,\ldots\}$ indexes the excited state. Since $T(h;E)$ was shown to decrease monotonically from ∞ to 0 as h ranges from 0 to ∞, it is again clear that each $E < 0$ will yield exactly one candidate as a minimizer of E and again by appealing to our existence result the minimizing potential is now characterized.

G. Technical arguments concerning unbounded intervals: Passage from finite- to infinite-interval problems

As promised earlier, we now present the limiting arguments which prove our assertions about optimizers for $\Omega = \mathbb{R}$ or $\mathbb{R}^+$. We concentrate on the case of minimization on $\mathbb{R}$, the other cases being similar. Let $E_k^*(M;l)$ denote the minimal k th eigenvalue for the interval $[-l,l]$ with Dirichlet boundary conditions at both end points and with $M^p = \int_{-l}^{l} |V(t)|^p\,dt$ and let $E_{k-1}^*(M;\mathbb{R})$ be the corresponding function for $\mathbb{R}$ where now $M^p = \int_{-\infty}^{\infty} |V(t)|^p\,dt$. By a well-known argument using the min–max principle (essentially reproduced below), $E_k^*(M;l)$ is a decreasing function of l and hence $\lim_{l\to\infty} E_k^*(M;l)$ exists or is $-\infty$. We shall denote this limit by $E_k^*(M;l\to\infty)$.

Proposition III.6: $E_{k-1}^*(M;\mathbb{R}) = E_k^*(M;l\to\infty)$. Furthermore, the lower bounds given by (3.19) and (3.24) hold.

Proof: First, we show that $E_{k-1}^*(M;\mathbb{R}) \leqslant E_k^*(M;l\to\infty)$. To see this, consider the minimizing potentials $V_k^*(t;l)$ for the k th eigenvalue of the Dirichlet problem on $[-l,l]$. We extend these potentials to $t \in \mathbb{R}$ by defining the extension to be 0 off $[-l,l]$. The resulting operators H_V on $L^2(\mathbb{R})$ can now be seen to have $(k-1)$th eigenvalue less than or equal to $E_k^*(M,l)$ by applying the min–max principle (form version, see Reed–Simon,[21] Vol. IV) after observing that the extensions of the eigenfunctions of the finite-interval problem lie in the form domain of the operator H_V acting on $L^2(\mathbb{R})$. This proves $E_{k-1}^*(M;\mathbb{R}) \leqslant E_k^*(M;l\to\infty)$.

To show the reverse inequality, we argue by contradiction. Thus we suppose $E_{k-1}^*(M;\mathbb{R}) < E_k^*(M;l\to\infty)$. By the definition of $E_{k-1}^*(M;\mathbb{R})$, we can find a $V \in L^p(\mathbb{R})$ such that $E_{k-1}^*(V) < E_k(M;l\to\infty)$. Now since $C_c^\infty(\mathbb{R})$ is a core for H_V the min–max principle applies with the supremum and infimum taken over the intersection of $C_c^\infty(\mathbb{R})$ with the usual sets. Thus, in particular, we can find k linearly independent functions $\phi_1,\phi_2,\ldots,\phi_k \in C_c^\infty(\mathbb{R})$ such that

$$\sup_{\substack{\phi \in \text{span}\{\phi_1,\ldots,\phi_k\} \\ \|\phi\|_2 = 1}} (\phi, H_V\,\phi) < E_k^*(M;l\to\infty). \tag{3.77}$$

We now let $[-R,R]$ be an interval containing the supports of the ϕ_i's $(i = 1,\ldots,k)$ in its interior and define V_R as the potential V restricted to $[-R,R]$. Note that $\|V_R\|_p \leqslant \|V\|_p$ and finally that $E_k(V_R) < E_k^*(M;l\to\infty)$, which follows from Eq. (3.77) above and the min–max principle applied to H_{V_R}. But $E_k(V_R) \geqslant E_k^*(M;l=R) \geqslant E_k^*(M;l\to\infty)$ and we have arrived at a contradiction.

To eliminate the possibility that $E_k^*(M;\mathbb{R}) = -\infty$, i.e., that

$$\inf_{\substack{\|V\|_p \leqslant M \\ V \in L^p(\mathbb{R})}} E_k(V) = -\infty,$$

and to assist with our characterization of minimizers we compute the limiting form as $l \to \infty$ of the relation between E^* and M for the minimization problem on $[-l,l]$ with Dirichlet boundary conditions. For this part of the argument we shall view E as fixed and compute the limiting value of M as $l \to \infty$. We consider here only the ground state. We have

$$\begin{aligned} M^p &= \int_{-l}^{l} |V(t)|^p\,dt \\ &= \int_{-l}^{l} |u(t)|^{2p/(p-1)}\,dt \\ &= 2\int_0^{u_1} \frac{q^{2p/(p-1)}}{\sqrt{2}(h - W(q;E))}\,dq, \end{aligned} \tag{3.78}$$

where we have changed variables to $q = u(t)$ and the new upper limit of integration $u_1 = u_1(h)$ is the positive turning point of the motion of the classical oscillator (recall that $h > 0$ in this problem). To take the limit as $l \to \infty$, observe that as l approaches infinity h decreases to 0 so it suffices to consider the limit of the expression above as $h \to 0^+$. Note, too, that as $h \to 0^+$, u_1 decreases monotonically to $u_1(0)$, the positive turning point when $h = 0$. We claim that as $h \to 0^+$

$$\begin{aligned} M^p &\to 2\int_0^{u_1(0)} \frac{q^{2p/(p-1)}}{\sqrt{(-E)q^2 - [2/(\alpha+1)]q^{\alpha+1}}}\,dq \\ &= \frac{p^p(-E)^{(2p-1)/2}}{(p-1)^{p-1}} B\left(p,\frac{1}{2}\right). \end{aligned} \tag{3.79}$$

To see this, we break up the interval $[0,u_1(h)]$ into two subintervals, $[0,u_1(0)]$ and $[u_1(0), u_1(h)]$. On $[0, u_1(0)]$, the integrand in Eq. (3.78) increases pointwise to that in Eq. (3.79) as h decreases to 0. As for the other part, we transform the integral to

$$2u_1(h)^{2p/(p-1)} \int_{u_1(0)/u_1(h)}^{1} \frac{s^{2p/(p-1)}}{\sqrt{[2/(\alpha+1)]u_1^{\alpha-1}(1-s^{\alpha+1}) - (-E)(1-s^2)}}\, ds \tag{3.80}$$

and, observing (by using Taylor's theorem on the expression under the radical) that the integrand is bounded by a constant times $(1-s)^{-1/2}$ for s near 1 and h near 0 while the length of the interval of integration shrinks to 0, we see that this quantity goes to 0 as $h \to 0^+$. Now the limiting relation between M and E represented by Eq. (3.79) is identical to that given by Eq. (3.18). This shows that the solutions [Eq. (3.15)] exhibited earlier in this section are indeed minimizers since they satisfy the characterizing equation (3.1) and they attain the minimal E allowable for the given M. □

The considerations above could also be applied to higher eigenvalues and to optimization problems on $\mathbb{R}^+$ with a variety of boundary conditions imposed at $t = 0$. In particular, all the lower bounds exhibited earlier can be demonstrated in this way. Note, too, that the procedure we applied above allows one to find the optimal bounds for eigenvalues whether or not an optimizing potential exists. When such a potential does exist we can find it using the characterizing equation (3.1) in the manner used above.

H. Concluding remarks

In conclusion, we would like to emphasize what we believe to be the wide applicability of the techniques and results presented above. In fact, there are a great variety of boundary conditions not dealt with above to which the methods are applicable. Furthermore, one could consider a different base (unperturbed) operator $H_0 = -d^2/dt^2 + W(t)$ to be perturbed to an operator $H_V = H_0 + V$ where V obeys an L^p constraint. Yet another direction which could be pursued in this context are the finite-interval optimization problems subject to periodic or antiperiodic boundary conditions. This problem cannot yet be treated by the methods described above since one potentially has a problem with degeneracy of the optimized eigenvalue which renders Proposition II.6 useless (except in the case of the ground state for periodic boundary conditions).

Note added: Since writing the preprint version of this paper, we have learned of additional related work on similar problems, using other methods. Specifically, we mention the work of Egnell,[42] Essén,[43] Keller,[44] and Melentsova.[45]

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An application of filtering theory to parameter identification using stochastic mechanics

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An estimation method for unknown parameters in the initial conditions and the potential of a quantal system using the stochastic interpretation of quantum mechanics and some results in system theory are presented. According to this interpretation the possible trajectories of a particle through coordinate space may be represented by the realization of a stochastic process that satisfies a stochastic differential equation. The drift term in this equation is derived from the wave function and consequently contains all unknown parameters in the initial conditions and the potential. The main assumption of the paper is that a continuous sequence of position measurements on the trajectory of the particle can be identified with a realization of this stochastic process over the corresponding period of time. An application of the stochastic filtering theorems subsequently provides a minimum variance estimate of the unknown parameters in the drift conditional on this continuous sequence of measurements. As simple illustrations, this method is used to obtain estimates for the initial momentum of a free particle given measurements on its trajectory and to construct an estimator for the unknown parameters in a harmonic potential. It is shown that an optimal estimator exists if the stochastic processes are associated with a wave function from a potential of the Rellich type. In addition the *a posteriori* probability density of the parameters in the quantal system is calculated, assuming that all parameters involved prescribe a Rellich potential.

I. INTRODUCTION

Many problems in physics and chemistry require inverting experimental data in order to obtain estimates of unknown potentials. Most rigorous quantum mechanical approaches to inversion problems are based on the analytical properties of the wave equation, which is, however, not a measurable quantity. In this paper we approach the problem more directly by employing the measurable amplitude of the particles using the stochastic interpretation of quantum mechanics and then estimating the unknown quantities by means of system theory. Since the square of the absolute value of the wave function may be interpreted as the probability density of the position of a particle, it is possible to associate a stochastic variable with it such that its realizations correspond to the collection of all possible trajectories of the particle in coordinate space. It is known from stochastic mechanics that this variable satisfies a stochastic differential equation of the diffusion type with a drift that depends on the wave function.[1-8] The main assumption of this paper is that position measurements of a particle over a continuous period of time are equivalent to the realizations of this stochastic variable on the corresponding time interval.

The drift term in the diffusion equation for the random variable contains all the information of the initial wave function and the potential, so a realization of the stochastic variable introduced above depends on the unknown parameters in the quantal system. The inversion problem now reduces to finding an estimator for these parameters given this realization. This approach is detailed in Sec. II. From filtering theory it is known that the minimum varianced estimator of the unknown parameters at time s, referred to as a filter, is given, by the *a posteriori* mean conditional on the obtained realization.[9,10] In Sec. III we introduce a theorem, which shows that under an appropriate condition such a filter satisfies a stochastic integral equation known as the Fujisaki–Kallianpur–Kunita equation.[11-13] Under more restricted circumstances, the *a posteriori* mean can be calculated from a conditional probability density that satisfies a stochastic partial differential equation involving the observed realization as input.[11,14]

This approach is different from the parameter estimation method used in Ref. 15 though both approaches use filtering methods. This paper assumed that the only source of error was the noise term with a variance proportional to Planck's constant. If that inhomogeneous noise term were to vanish the observations would reduce to exact measurements on a Newtonian system, which is not the case in Ref. 15. There the measurement was assumed to be proportional to the quantum mechanical expectation and an inhomogeneous white noise process modeling the experimental error. If the variance of this inhomogeneous process approached zero, the observation would reduce to the quantum mechanical expectation. The various expressions in these two papers must therefore carry a different interpretation.

In Sec. IV the method is illustrated by two examples. We apply the filtering formalism to estimate the unknown initial momentum of a free particle by measurements on its trajectory. This case is of interest because it is related to the uncertainty principle. In addition we calculate the *a posteriori*

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probability density for two unknown parameters in a harmonic potential. In Sec. V we introduce a condition necessary for the existence of the Rao–Cramer lower bound[9,10] to the covariance matrix of the estimator, and we show that it can be calculated from the sensitivity equations of the quantum mechanical wave function.

In Sec. VI it is shown that for a certain class of potentials the estimator exists and is given by the solution to the Fujisaki–Kallianpur–Kunita integral equation. For the same class of potentials we present the analytical form of the *a posteriori* probability density for the unknown parameters in the quantal system using the extended Bayes formula.[11] In Sec. VII we summarize the paper and suggest an extension of the *a posteriori* probability density derived in Sec. VI for the case that the number of unknown parameters is infinite.

II. STOCHASTIC MECHANICS

This section briefly summarizes the relationship between quantum mechanics and stochastic mechanics and specifies the assumptions on the experimental observations that make it possible to represent the estimation of unknown parameters as a filtering problem. More detailed information on the subject of stochastic mechanics can be found in Refs. 1–8.

In a quantal system the probability $\rho[\mathbf{x},s]\Delta\mathbf{x}$ of finding the position of a particle in a volume element $\Delta\mathbf{x}$ around the point $\mathbf{x}$ in coordinate space at time s is equal to $\rho[\mathbf{x},s]\Delta\mathbf{x} = |\psi[\mathbf{x},s]|^2\Delta\mathbf{x}$, where $\psi[\mathbf{x},s]$ is the wave function satisfying the Schrödinger equation $i\hbar(\partial/\partial s)\psi[\mathbf{x},s] = \hat{H}\psi[\mathbf{x},s]$ with $x\in R^N$, $\hat{H} = -(\hbar^2/2m)\Delta + V$. The function $V = V(\mathbf{x})$ is the potential, Δ is the Laplacian in R^N, and $\rho[\mathbf{x},0] = |\psi[\mathbf{x},0]^2$ is the initial probability density. There exists a stochastic variable $\mathbf{x}(s)\in R^N$ associated with the probability density $\rho[\mathbf{x},s]$ such that for any Borel set A in R^N,

$$p[\mathbf{x}(s)\in A] = \int_A d\mathbf{x}\,\rho[\mathbf{x},s], \tag{2.1}$$

where $p[\Lambda]$ is the probability of the event Λ. The time evolution of the probability density $\rho[\mathbf{x},s]$ may be obtained from the Schrödinger equation, so the stochastic process defined in (2.1) depends on the potential in the Hamiltonian $\hat{H}$ in a complicated fashion.

The collection of possible trajectories on the interval $[0,s]$ is given by all possible realizations of the random variable $\mathbf{x}(s')$, $s'\in[0,s]$, and has a measure whose image at time s is given by (2.1). It has been shown in recent years[1–6] that the process $\mathbf{x}(s)$ satisfies the following stochastic differential equation:

$$d\mathbf{x}(s) = \mathbf{b}[\mathbf{x}(s),s]ds + \sigma\, d\mathbf{w}(s), \tag{2.2}$$

where $E[\mathbf{w}(s)] = 0$, $E[\mathbf{w}(s)\mathbf{w}^T(s')] = \min(s,s')$, $\sigma^2 = \hbar/m$, and $\mathbf{b}(s) = \mathbf{b}[\mathbf{x}(s),s]: R^N \to R^N$ so that $\mathbf{x}(s)$ becomes a diffusion process. The drift term $\mathbf{b}[\mathbf{x},s]$ is related to the wave function ψ in the following manner:

$$b[\mathbf{x},s] = \mathrm{Re}\left(\frac{\nabla\psi[x,s]}{\psi[\mathbf{x},s]}\right) + \mathrm{Im}\left(\frac{\nabla\psi[x,s]}{\psi[\mathbf{x},s]}\right), \tag{2.3}$$

where $\nabla = (\partial/\partial x_1,\ldots,\partial/\partial x_N)$. Notice that the wave function depends on the initial condition $\psi_0[\mathbf{x}]$ so that the drift in (2.3) contains all the information of the initial wave function $\psi_0[\mathbf{x}]$. The probability density associated with the radom variable in (2.3) is therefore not only determined by the initial distribution $\rho[\mathbf{x},0] = |\psi_0[\mathbf{x}]|^2$, but also depends on the phase of the initial wave function. Since ψ often has zeros, the drift term $b[\mathbf{x},s]$ may have singularities so that the stochastic equation (2.2) generally does not have a strong solution. In Sec. VI we will elaborate on the existence of the solution to Eq. (2.2) and its associated measure.

If a single experimental observation on a quantal system is performed to determine the position of a particle at time s, the measurement ideally results in a realization of the stochastic variable $\mathbf{x}(s)$ defined in Eq. (2.2). Similarly, a continuous series of observations that do not disturb the particle measure its trajectory over a period of time s, and the result is equivalent to a realization of the random process $\{\mathbf{x}(s')\}_{0<s'<s}$.

To demonstrate how filtering theory is now used to establish the parameters in the quantal system, consider the wave function to be dependent on a vector of unknown parameters $\gamma\in R^K$. They can reside in the initial wave function or in the potential so that $V = V(\gamma)$. As a consequence of (2.3), the drift $\mathbf{b}[\mathbf{x},s]$ depends on γ and can be written as $\mathbf{b} = \mathbf{b}[\mathbf{x}(s),\gamma,s]$. The vector of parameters is time independent so the combined equations for the vector γ and the stochastic process $\mathbf{x}(s)$ can be written as

$$\frac{d}{ds}\gamma = 0, \tag{2.4a}$$

$$d\mathbf{x}(s) = \mathbf{b}[\mathbf{x}(s),\gamma,s] + \sigma\, d\mathbf{w}(s), \tag{2.4b}$$

which are usually referred to in system theory as state and observational equations, where the parameter vector in (2.4a) is defined as the (unknown) state of the system and where the process $\mathbf{x}(s)$ is the observable variable. Using the filtering theorems below, an estimate of the parameters γ at time s can be obtained from the realization $\{\mathbf{x}(s')\}_{0<s'<s}$.

It is possible that the parameters γ are influenced by physical processes that have a random character and are not part of the original model (e.g., the potential may be stochastic). Another possibility is that some of the N processes $x_1(s),\ldots,x_N(s)$ in (2.4b) are unobservable and consequently have to be added to the state of the system (2.4a). The enlarged state is denoted $\gamma(s)$, and the state and observational equations in their most general form become

$$d\gamma(s) = \mathbf{h}[\mathbf{x}(s),\gamma(s),s]ds + \mathsf{P}\, d\mathbf{w}_1(s), \tag{2.5a}$$

$$d\mathbf{x}(s) = \mathbf{b}[\mathbf{x}(s),\gamma(s),s]ds + \sigma\, d\mathbf{w}_2(s), \tag{2.5b}$$

where $\gamma(s)\in R^K$, and where $\mathbf{h}(s) = \mathbf{h}[\mathbf{x}(s),\gamma(s),s]$: $R^K \to R^K$. The matrix P is of appropriate dimension and specifies the magnitude of the stochastic fluctuations while $\mathbf{w}_1(s)$ and $\mathbf{w}_2(s)$ are independent Wiener processes of dimension K and N, respectively. The purpose again is to estimate $\gamma(s)$ from the information $\{\mathbf{x}(s)\}_{0<s'<s}$.

In Sec. III we introduce the equations of filtering theory that are relevant for the solution of the state estimation problem posed in (2.4) and (2.5).

III. STOCHASTIC FILTERING THEORY

As is well known in the filtering literature, the minimum variance estimate of the nonmeasurable variables $\gamma(s)$ in (2.5a) is the *a posteriori* mean conditional on the realization of the measurable variables $\mathbf{x}(s)$ on $[0,s]$; $E[\gamma(s)|\{\mathbf{x}(s)\}_{0\leqslant s\leqslant t}]$. This estimator satisfies the Fujisaki–Kunita–Kallianpur integral equation introduced below and can be obtained from the *a posteriori* probability density, which under more restricted conditions satisfies the Kushner equation in Theorem III.2.

We assume that in (2.5) the drifts $\mathbf{h}(s)=\mathbf{h}[\mathbf{x}(s),\gamma(s),s]$ and $\mathbf{b}(s)=\mathbf{b}[\mathbf{x}(s),\gamma(s),s]: R^K\to R^K$ are such that

$$\int_0^t ds\, E|\mathbf{h}(s)|^2<\infty, \quad \int_0^t ds\, E|\mathbf{b}(s)|^2<\infty, \tag{3.1}$$

where the expectation E is over the random processes introduced above. Then we have that the following theorem holds.

Theorem III.1: Let $F_s^{\mathbf{x}}$ be the sigma algebra generated by the stochastic process $\mathbf{x}(s')$, $0\leqslant s'\leqslant s$, and define the process $\boldsymbol{\nu}_s$,

$$d\boldsymbol{\nu}_s = d\mathbf{x}(s) - E[\mathbf{b}(s)|F_s^{\mathbf{x}}]ds, \quad 0\leqslant s\leqslant t. \tag{3.2}$$

Then if condition (3.1) holds, the estimator $E[\gamma(s)|F_s^{\mathbf{x}}]$ for the state $\gamma(s)$ in (2.5a) given the realization $\{\mathbf{x}(s)\}_{0\leqslant s'<s}\in F_s^{\mathbf{x}}$ from (2.5b) satisfies the integral equation[11–13]

$$\begin{aligned}E[\gamma(s)|F_s^{\mathbf{x}}] &= E[\gamma(0)|F_0] + \int_0^s d\tau\, E[\mathbf{h}(\tau)|F_\tau^{\mathbf{x}}] \\ &\quad + \frac{1}{\sigma^2}\int_0^s \{E[\gamma(\tau)\cdot\mathbf{b}(\tau)^T|F_\tau^{\mathbf{x}}] \\ &\quad - E[\gamma(\tau)|F_\tau^{\mathbf{x}}]\cdot E[\mathbf{b}(\tau)|F_\tau^{\mathbf{x}}]^T\}\cdot d\boldsymbol{\nu}_\tau,\end{aligned} \tag{3.3}$$

where F_0 is the sigma algebra generated by the random variable $\mathbf{x}(0)=\mathbf{x}_0$. For the proof see Ref. 10, Theorem 8.1.

Notice that the existence of the estimator does not have additional requirements on the sigma algebra $F_s^{\mathbf{x}}$. From (3.1) it follows that $\mu_\gamma \ll \mu_{\mathbf{w}_1}$ and $\mu_{\mathbf{x}} \ll \mu_{\mathbf{w}_2}$, where μ_γ, $\mu_{\mathbf{x}}$, $\mu_{\mathbf{w}_1}$, $\mu_{\mathbf{w}_2}$ are the measures associated with the processes $\gamma(s)$, $\mathbf{x}(s)$, $\mathbf{w}_1(s)$, $\mathbf{w}_2(s)$, respectively.[11] The inverse relation is, however, not necessary for the theorem.

The conditional mean $E[\mathbf{b}(s)|F_s^{\mathbf{x}}]$ may be calculated from the *a posteriori* probability distribution $p[\gamma',s] = p[\gamma'|F_s^{\mathbf{x}}]$, $\gamma'\in R^K$, i.e., the probability density of the state $\gamma(s)$ given the observations $\mathbf{x}(s')$, $0\leqslant s'\leqslant s$. If additional requirements are added to condition (3.1) it is possible to derive the following equations, (3.4) and (3.5), for $p[\gamma',s]$.

Theorem III.2: Assuming that (3.1) holds then under certain restrictions on the operator L_s^* and the process $\boldsymbol{\nu}_s$, the density $p[\gamma',s]$ for the state $\gamma(s)$ in (2.5a) given the realization $\{\mathbf{x}(s)\}_{0\leqslant s'\leqslant s}$ satisfies the following stochastic equation[9,11,14]:

$$\begin{aligned}dp[\gamma',s] &= L_s^* p[\gamma',s]ds + (1/\sigma^2)p[\gamma',s]\{\mathbf{b}(s) \\ &\quad - E[\mathbf{b}(s)|F_s^{\mathbf{x}}]\}^T\cdot d\boldsymbol{\nu}_s, \quad 0\leqslant s\leqslant t,\end{aligned} \tag{3.4}$$

where

$$E[\mathbf{b}(s)|F_s^{\mathbf{x}}] = \int_{R^K} d\gamma'\, p[\gamma',s]\mathbf{b}[\mathbf{x}(s),\gamma',s]. \tag{3.5}$$

For a proof of the Kushner equation (3.4), see Ref. 11, Chap. 8.

The first term on the right-hand side of Eq. (3.4) involves the Fokker–Planck operator L^* associated with the stochastic equations (2.5a) and propagates the probability distribution in time as if no information has been obtained. The second part on the right-hand side of (3.4) contains the information of the observations $\{\mathbf{x}(s)\}_{0\leqslant s'\leqslant s}$ embedded in the process $\boldsymbol{\nu}_s$. Equation (3.4) is a stochastic partial differential equation that has to be interpreted in the sense of Ito.

In Sec. IV we illustrate our approach by applying the filtering method to estimate the unknown initial momentum of a free particle and we provide an estimator for the unknown parameters in a harmonic potential.

IV. APPLICATIONS

In the first example we obtain an estimate for the initial momentum of a free particle [γ in (2.4a)] given an observed trajectory in coordinate space $\{x(s)\}_{0\leqslant s\leqslant t}$, where $x(s)$ satisfies (2.4b), $K=N=1$. A filter exists even if the initial probability density is not normalizable. In Sec. IV B we construct the *a posteriori* probability density for the unknown parameters in a harmonic potential using similar information.

A. Estimation of the momentum of a free particle by position measurement

Consider a free particle with the potential $V\equiv 0$ and the initial condition

$$\psi[x,0] = \frac{1}{(\delta\sqrt{\pi})^{1/2}}\exp\left[-\frac{x^2}{2\delta^2} + i\frac{\gamma x}{\hbar}\right], \tag{4.1}$$

then the wave function ψ evolves in time as

$$\begin{aligned}\psi[x,s] &= \frac{1}{(\delta\sqrt{\pi})^{1/2}}\frac{1}{(1+is)^{1/2}}\exp\left[\frac{i(\gamma x - \gamma^2 s/2m)}{\hbar}\right] \\ &\quad \times\exp\left[-\frac{(x-\gamma s/m)^2}{\delta^2}\cdot\frac{1-is}{1+is}\right].\end{aligned} \tag{4.2}$$

The distribution for the initial position of the particle, $|\psi[x,0]|^2$, is a Gaussian with a variance of $\frac{1}{2}\delta^2$ and zero mean, where the parameter γ is the initial phase, or momentum, which is assumed to be unknown. From (2.3) it is easily seen that for this choice of initial condition the drift $b[x,s]$ becomes linear so that (2.4b) reduces to

$$dx(s) = [\gamma/m + \alpha(s)\{x(s) - (\gamma/m)s\}]ds + \sigma\, dw(s), \tag{4.3}$$

where

$$\alpha(s) = \kappa[(\kappa s - 1)/(\kappa^2 s^2 + 1)], \quad \kappa = \hbar/m\delta^2. \tag{4.4}$$

Since γ is time independent, Eq. (2.4a) holds, and identifying (4.3) and (2.4b) it is clear that γ can be estimated from the realization $\{x(s)\}_{0\leqslant s'\leqslant s}$ by means of applying the general methods of Sec. III. Both equations (2.4a) and (2.4b) are linear and it can be shown that in this case the distribution for the parameter γ conditional on the experi-

mental data $\{x(s')\}_{0\le s'<s}$ is a Gaussian, which can be specified by its first two moments.[9,11,14] Substituting this Gaussian into Eq. (3.4) leads to two equations describing the time evolution of its mean and variance, known as the Kalman-filtering equations.[11,16] From these we find that the optimal estimate $\hat{\gamma}(s) = E[\gamma|\ \{x(s')\}_{0\le s'<s}]$ of γ and its variance $V_\gamma(s) = \mathrm{Var}(\hat{\gamma}(s))$ satisfy

$$d\hat{\gamma}(x) = \frac{mV_\gamma(s)[1-s\alpha(s)]}{\hbar} \times\left[dx(s) - \frac{(1-s\alpha(s))}{m}\hat{\gamma}(s) - \alpha(s)x(s)\right], \tag{4.5a}$$

$$\frac{d}{ds}V_\gamma(s) = -\frac{V_\gamma(s)^2}{m\hbar}[1-s\alpha(s)]^2. \tag{4.5b}$$

The equation for the estimator is linear and can be solved in terms of the observed sequence $x(s')$, $0\le s'\le s$ once $V_\gamma(s)$ is known. The equation for the variance of the estimator, (4.5b), is of the Riccati type and is independent of the data due to the linear nature of the estimation problem. It can be easily solved to yield

$$V_\gamma(s) = \left(\frac{1}{V_0} + \frac{1}{m\hbar}\int_0^s d\tau\,[1-\tau\alpha(\tau)]^2\right)^{-1}, \tag{4.6}$$

where $V_\gamma(0) = V_0$. As time approaches infinity it is easy to see that

$$V_\gamma(s)\to V_\infty = \left[\frac{1}{V_0} + \frac{\delta^2}{\hbar^2}\left(\frac{\pi}{2}+1\right)\right]^{-1}, \tag{4.7}$$

so that after an infinite amount of measurements the variance of the optimal estimate approaches a finite limit. *The initial phase can therefore not be determined without error.*

The *a priori* knowledge about γ is represented by the initial estimate $\hat{\gamma}(0)$ and variance V_0. As the available foreknowledge decreases, $V_0\to\infty$, we see from (4.7) that $V_\gamma(s)\uparrow V_\infty < \infty$; hence, even in the case that no initial information is available ($V_0 = \infty$), an estimator exists and has finite variance. In this case, $V_\infty \approx 0.6\,\hbar^2/\delta^2$ so that the final variance is inversely proportional to the variance of the free particle at the beginning of the measurement process. Finally, if the position of the particle at time zero is very accurately determined, say $\delta^2 \ll \hbar^2/V_0$, then we see that $V_\infty \approx V_0$ so that almost no information can be gained from the observations, and if the initial position becomes infinitely precise, $\delta\to 0$, it becomes impossible to obtain any information ($V_\infty = V_0$).

The uncertainty principle states that it is impossible to determine the momentum and the position of a particle both to an arbitrary degree of accuracy. The result derived above is therefore consistent with quantum mechanics, and it shows that even from an infinite sequence of measurements on the position of a particle, no information can be obtained about the momentum γ if the initial position of the particle is known to infinite accuracy. So far we assumed, obviously, that the system was not meaningfully disturbed by the position measurements, which is not entirely correct; precise measurements will generally alter the quantal system. Usually only one measurement can be performed at a fixed time or the time interval for measurement remains short. The result above, however, is of interest as a theoretical limit and further work in this area is warranted.

A closely related case is when we consider the wave function of a free particle such that $\psi[x,s] = \exp[-Ax + iBs]$, where $A = \gamma/m\sigma^2$, $B = \gamma^2/(m\sigma)^2$, the unknown parameter γ being the initial momentum of the particle. This probability density is not normalized but the associated stochastic process (2.4b) still exists. Indeed the drift $b[x,s]$ for the process equals $b[x,s] = \gamma/m$ and the *a posteriori* probability density becomes a Gaussian with the following mean and variance:

$$\hat{\gamma}(s) = E[\gamma|F_s^x] = m\frac{(x(s)-x(0))}{s}, \qquad \mathrm{Var}(\hat{\gamma}) = \left(2\pi\frac{\hbar m}{s}\right)^{1/2}. \tag{4.8}$$

It is interesting to notice that in this case the variance approaches zero as $s\to\infty$. Hence, in constrast to the previous example, for the case of the free particle where no information exists for its initial position ($\delta\to\infty$), the initial momentum γ can be determined exactly if the position measurements are continued for an infinite amount of time. Since γ is related to the initial momentum we find that the initial energy is proportional to γ^2. An estimate of the initial energy of the particle is then $E[\gamma^2|F_s^x]/2m$ and can be calculated from (4.8). In fact,

$$E[\gamma^2|F_s^x]/2m = m[\{x(s)-x(0)\}^2 + \hbar^2]/2s^2. \tag{4.9}$$

Notice that the energy estimator is not just given by $\hat{\gamma}(t)^2/2m$ but also contains a term that decreases with time like $1/s^2$ and is proportional to $\hbar^2$.

B. Estimation of a harmonic potential from position measurements

A more complicated situation is where the particle moves in the presence of a potential well, where in this case the potential is a one-dimensional harmonic oscillator $V = \gamma_1 x^2 + \gamma_2 x$, with the parameters being unknown. From the realization of the associated random variable we now construct the estimates for the two parameters as follows. Suppose that the initial wave function has the general form $\psi[x,0] = \exp[A_0x^2 + B_0x + C_0 + i\{E_0x + F_0\}]$, then from the Schrödinger equation we see that $\psi[x,s] = \exp[Ax^2 + B(s)x + C(s) + i\{E(s)x + F(s)\}]$, where the functions $B(s)$, $C(s)$, $E(s)$, and $F(s)$ satisfy the following (linear) differential equations:

$$\frac{d}{ds}B(s) + 2\sigma^2E(s) = 0,\quad \frac{d}{ds}C(s) + \sigma^2B(s)E(s) = 0,$$
$$\frac{d}{ds}F(s) - 2\sigma^2\{B(s)^2\} = 0, \tag{4.10}$$
$$\frac{d}{ds}E(s) + \frac{\gamma_2}{m\sigma^2} - 2\sigma^2AB(s) = 0,$$

where $\sigma^2 = \hbar/m$, $A^2 = \gamma_1/2m\sigma^4$, $B(0) = B_0$, $C(0) = C_0$, $E(0) = E_0$, and $F(0) = F_0$. These equations can be found from substituting the wave function into the Schrödinger equation.

Using (2.3) the associated drift may be shown to become $b[x,s] = 2Ax + R$, where $A = A[\gamma]$, $R = R[\gamma] = B(s) + E(s)$, $\gamma = (\gamma_1,\gamma_2)$. The functions $B(s)$ and $E(s)$

and the constant A generally depend on γ_1 and γ_2 in a nonlinear fashion. As usual the time independent parameters in γ are identified with the state of the system (2.4a) and then using this drift, Eq. (2.4b) becomes linear. The *a posteriori* probability density for γ, given the observations $p[\gamma'|F_s^x]$, satisfies Eq. (3.4), and using the method of characteristics[9] the solution is given by

$$p[\gamma'|F_s^x] = z[\gamma']\exp\left[\frac{1}{\sigma^2}\int_0^s b(\tau)dx(\tau) - \frac{1}{2\sigma^2}\int_0^s d\tau\, b(\tau)^2\right] \times\left\{\int d\gamma\, z[\gamma']\exp\left[\frac{1}{\sigma^2}\int_0^s b(\tau)dx(\tau) - \frac{1}{2\sigma^2}\int_0^s d\tau\, b(\tau)^2\right]\right\}^{-1}, \tag{4.11}$$

where $b(\tau) = b[x(\tau),\gamma',\tau]$ is the drift term introduced above and where the probability density $z(\gamma')$ is the *a priori* information on the parameters.

For example, suppose that $\gamma_2 = 0$ so that only the unknown constant γ_1 needs to be estimated. As time increases the optimal estimate approaches the maximum of the density (4.11) (the maximum likelihood estimate) so that

$$\hat{\gamma}_1(s) \approx 2m\sigma^4\left[\left(\int_0^s x(s')dx(s') - 2\int_0^s x(s')R\,[s']ds'\right) \times\left(2\int_0^s x(s')^2\,ds'\right)^{-1}\right]^2 \approx 2m\sigma^4\left[\frac{4}{s\sigma^2}\int_0^s x(s')^2\,ds\right]^{-2} \tag{4.12}$$

as time approaches infinity. The average $(1/s)\times\int x(s')^2ds' \to \sigma^2/4A$ for large s and has a variance that decreases as $1/s$. From Eq. (4.12) it then follows that as time increases $\hat{\gamma}_1$ converges to the actual parameter $\gamma_1 (P - as)$ and that its variance also decreases with the time of observation.

Expression (4.11) is more generally valid for drifts $\mathbf{b}(s) = b[\mathbf{x}(s),\gamma',s]$ that satisfy the requirements of Theorem 3.2 but the usual assumptions introduced to validate the Kushner equation do not hold for (2.4b) or (2.5b).[11] We will say more about the use of this equation in Sec. VII.

In Sec. V we present a lower bound to the covariance matrix of the estimator, which is particularly useful in determining its long-time behavior.

V. ASYMPTOTIC ANALYSIS

It can be shown that if certain conditions are satisfied the covariance matrix of the estimator of the parameters $\gamma_1,\ldots,\gamma_K$ in (2.4a) asymptotically approaches the inverse of the associated Rao–Cramer lower bound as time increases to infinity.[9,10] The rank of the Rao–Cramer matrix also shows whether the observations under consideration can determine all parameters independently and the diagonal elements of the inverse of the Rao–Cramer bound generally provide information on the rate with which information is gained on a parameter as further observations are obtained.

Using Ref. 10 the Rao–Cramer inequality for the covariance matrix of a multidimensional estimator can be found; however, the existence of the Rao–Cramer lower bound matrix is not guaranteed in the present case. In this section we introduce a condition that will ensure the existence of the Radon–Nikodym derivative necessary to calculate the lower bound matrix so that the derivation of the inequality can proceed analogous to the method in Ref. 10. We also show that the Rao–Cramer matrix can be calculated from the sensitivity equations of the Schrödinger equation.

Henceforth we assume that the drift $\mathbf{b}(s) = \mathbf{b}[\mathbf{x}(s),\gamma,s]$ is obtained from the wave function $\psi = \psi[\mathbf{x},\gamma,s]$ for every $\gamma \in R^K$ and that it is a square integrable random process for every choice of vector parameter γ. This means that

$$\int_0^t ds\, E'[\mathbf{b}[\mathbf{x}(s),\gamma,s]^2] = \int_0^t ds\int_{R^N} d\mathbf{x}|\psi|^2|\nabla\log\psi|^2 = \int_0^t ds\int_{R^N} d\mathbf{x}|\nabla\psi|^2 < \infty, \tag{5.1}$$

where E' is the expectation only over the random variable $\{\mathbf{x}(s)\}_{0\leqslant s\leqslant t}$ in contrast to (3.1), where the expectation E extends to all stochastic variables. The equalities can be found from calculating the drift term using (2.3) and substituting the result into (5.1). This condition on $\mathbf{b}(s)$ is equivalent to requiring that the drift be generated by a wave function associated with a finite energy for every choice of $\gamma \in R^N$.

An important consequence of (4.1) is the following theorem, related here without proof.[10]

Theorem V.1: Consider the observational equation (2.4b) and define $d\boldsymbol{\eta}(s) = \sigma\, d\mathbf{w}(s)$, $s \geqslant 0$. Let the measure $\mu_{\mathbf{x}}$ be associated with the process $\mathbf{x}(s)$ that satisfies (2.4b) with $\mathbf{b}(s) = \mathbf{b}[\mathbf{x}(s),\gamma,s]$. Then, for the Radon–Nikodym derivative $(d\mu_{\mathbf{x}}/d\mu_{\boldsymbol{\eta}})(\boldsymbol{\eta},\gamma,s)$ of the measure $\mu_{\mathbf{x}}$ with respect to the measure $\mu_{\boldsymbol{\eta}}$, we find

$$\frac{d\mu_x}{d\mu_\eta}(\boldsymbol{\eta},\gamma,s) = \exp\left[\frac{1}{\sigma^2}\Gamma_s(\mathbf{b}(s)) - \frac{1}{2\sigma^2}\int_0^s d\tau\,\mathbf{b}(\tau)^2\right], \quad 0\leqslant s\leqslant t, \tag{5.2}$$

where the drift is evaluated as $\mathbf{b}(s) = \mathbf{b}[\mathbf{n},\gamma,s]$ and where

$$\Gamma_s(\mathbf{b}(s)) = \text{p-lim}_n\left[\chi_{\{\int_0^s d\tau\,\mathbf{b}(\tau)^2<\infty\}}\int_0^s z_n[\boldsymbol{\eta}]^T\cdot d\boldsymbol{\eta}(\tau)\right]. \tag{5.3}$$

Here $\mathbf{z}_n$ is a sequence of functions such that

$$\text{p-lim}_n\left[\chi_{\{\int_0^s ds\,\mathbf{b}(\tau)^2<\infty\}}\int_0^s d\tau(\mathbf{b}(\tau) - \mathbf{z}_n)^2\right] = 0 \tag{5.4}$$

with $\chi_A(x) = 1$ if $x \in A$ and is 0 elsewhere. Also, p-lim$_n$ denotes convergence in probability, i.e., for random variables ξ_n, ξ, p-lim$_n\,\xi_n = \xi$ is equivalent to the statement that for all $\delta > 0$, $p[|\xi_n - \xi| > \delta] \to 0$ as $n \to \infty$.

In addition, for s, $0 \leqslant s \leqslant t$,

$$\frac{d\mu_x}{d\mu_\eta}(\mathbf{x},\gamma,s) = \exp\left[\frac{1}{\sigma^2}\int_0^s \mathbf{b}(\tau)^T\cdot d\mathbf{x}(\tau) - \frac{1}{2\sigma^2}\int_0^s d\tau\,\mathbf{b}(\tau)^2\right] \tag{5.5}$$

if $\mathbf{b}(s)$ is evaluated as $\mathbf{b}(s) = b[\mathbf{x},\gamma,s]$.

Now the existence of the Radon–Nikodym derivative has been assured by condition (5.1), the Rao–Cramer lower bound matrix can be constructed. Define a vector of func-

tionals $\nu_j(\mathbf{x})$: $\{\mathbf{x}(s')\}_{0<s'<s} \to R$, $j = 1,...,K$, where

$$\nu_j(\mathbf{x}) = \frac{\partial}{\partial \gamma_j} \log \frac{d\mu_x}{d\mu_\eta}(\mathbf{x},\gamma,s), \quad j = 1,...,K, \tag{5.6}$$

and let the matrix Z be defined as $Z = E'[\nu\nu^T]$. An estimator of the parameter vector γ is a functional $\phi \in R^K$, ϕ_j: $F_s^x \to R^K$, $j = 1,...,K$, where F_s^x is the sigma algebra of events $\{\mathbf{x}(s)\}_{0<s'<s}$ with a covariance matrix $\mathsf{R} = E[\phi\phi^T] - E[\phi]E[\phi]^T$. Using the arguments in Ref. 14 it can now be shown that for any collection of functionals $\phi = (\phi_1,...,\phi_K)$ (i.e., any collection of estimators) we have that the matrix combination $\mathsf{R} - \mathsf{A}\mathsf{Z}^{-1}\mathsf{A}^T$ is positive definite, or $\mathsf{R} - \mathsf{A}\mathsf{Z}^{-1}\mathsf{A}^T \geqslant 0$. Here $\mathsf{A} = E'[\phi\nu^T] - E[\phi]E'[\nu]^T = E'[\phi\nu^T]$ since $E'[\nu] = 0$.

Using (5.6) we find for the matrix elements of the Rao–Cramer matrix Z,

$$(\mathsf{Z})_{1k} = E[\nu_1\nu_k] = \frac{1}{\sigma^2} E'\left[\int_0 d\tau \frac{\partial}{\partial \gamma_1}\mathbf{b}(\tau)^T \cdot \frac{\partial}{\partial \gamma_k}\mathbf{b}(\tau)\right], \tag{5.7}$$

so that the matrix Z can be expressed in terms of the wave function via (2.4a). Indeed, we have

$$\frac{\partial}{\partial \gamma_j} b_i(s) = (\mathrm{Im} + \mathrm{Re}) \frac{\partial^2}{\partial x_i \partial \gamma_j} \log \psi[\mathbf{x},s], \tag{5.8}$$

which can be calculated from the sensitivity equation

$$i\hbar \frac{\partial}{\partial s}\left(\frac{\partial \psi}{\partial \gamma_j}\right) = -\frac{\hbar^2}{2m}\Delta \frac{\partial \psi}{\partial \gamma_j} + V\frac{\partial \psi}{\partial \gamma_j} + \psi \frac{\partial V}{\partial \gamma_j}. \tag{5.9}$$

If the covariance matrix of an estimator asymptotically approaches the inverse of the Rao–Cramer lower bound matrix Z, as time approaches infinity, the estimator is referred to as asymptotically efficient. Some conditions necessary for asymptotic efficiency are known,[9,10] but no work on this particular case has been done.

Though the drift terms in (2.4b) and (2.5b) may be highly nonlinear, we show in Sec. VI that an estimator for the parameters exists if the potential V satisfies certain general requirements.

VI. PROOF OF EXISTENCE OF THE PARAMETER ESTIMATOR

In this section we argue that the optimal estimator for $\gamma(s)$ in (2.5a), given a realization of (2.5b) on the interval $[0,s]$, exists if all drift terms in (2.5) are generated by a Rellich potential or, more generally, if the total (average) energy in the quantal system is finite. We also show the exact form for the *a posteriori* probability density of the parameter vector γ in (2.4a) given the realization $\{\mathbf{x}(s)\}_{0<s<t}$ from (2.4b). In Sec. VII it is speculated that a similar analytical formula can be derived if (2.4b) is cast in a functional form.

It was proven by Carlen[8] that a (weak) solution to (2.2) exists if the potential V in the Schrödinger equation is of the Rellich type. This means that an outcome space, a measure, and a sigma algebra exist such that (2.2) holds if the potential V has the following properties.

(1) As a multiplication operator, the domain of V contains the domain of the operator Δ, the Laplacian in R^N.

(2) For some $a < 1$ and b in R, for all functions f that belong to the domain of Δ, we have $\|Vf\| \leqslant a\|\tfrac{1}{2}\Delta f\| + b\|f\|$ ($\|\cdot\|$ is an L^2 norm). Many common potentials are Rellich type potentials. For instance, the Coulomb potential is a Rellich potential and in R^3 all square integrable potentials or finite potentials are of the Rellich type (see also Sec. VII).

Via the Kato–Rellich theorem and Stone's theorem, Carlen[8] established the existence of the Markovian propagator for the backward equation associated with (2.2) and it was also shown that (i) the condition (3.1) holds for the drift term (2.3) if ψ is generated by a Rellich potential, and (ii) a measure μ_x and a sigma algebra F_s^x exists such that $\mathbf{x}(s)$ satisfies Eq. (2.2). The process $\mathbf{x}(s)$ is a square integrable Markov process with a jointly measurable version. The image of the measure under $\mathbf{x}(s)$ has the probability density $\rho[\mathbf{x},s] = |\psi[\mathbf{x},s]|^2$.

The existence of the measure μ_x and the sigma algebra F_s^x [i.e., the collection of events generated by the process $\mathbf{x}(s)$] for Rellich potentials could also have been established by relating them to the Wiener measure μ_w and the sigma algebra F_s^w [i.e., the collection of events generated by the Wiener process $\mathbf{w}(s)$] using Theorem V.1. For Rellich potentials condition (3.1) is satisfied so this theorem implies that the measure μ_x of the process $\mathbf{x}(s)$ in (2.2) is absolutely continuous with respect to the measure μ_η, i.e., $\mu_x \ll \mu_\eta$, where $d\eta(s') = \sigma\, d\mathbf{w}(s')$, $0 \leqslant s' \leqslant s$, consequently they can be related via the Radon–Nikodym derivative (5.2). It has been shown[5] that the stochastic process $\mathbf{x}(s)$ does not cross the singularities in the drift $\mathbf{b}[\mathbf{x},s]$. The collection of paths that has this property has a positive Wiener measure so the sigma algebra F_s^x generated by the process $\mathbf{x}(s')$ is a proper sub-sigma algebra of F_s^η.

The conclusions above can be applied to (2.5a) and (2.5b) so if the drift terms $\mathbf{b}(s)$ and $\mathbf{h}(s)$ are jointly generated by a Rellich potential it is true that a solution to the stochastic differential equations (2.5a) and (2.5b) exists. Condition (3.1) is also satisfied, so from Theorem 3.1 it follows that the estimator $\hat{\gamma}(s) = E[\gamma(s)|F_s^x]$ exists and that it satisfies the Fujisaki–Kallianpur–Kunita equation (3.3). This remains true for any drift term $\mathbf{h}(s)$ in (2.5b) satisfying (3.1). To use the arguments above in order to establish existence of the estimator of γ in (2.4a) it is not enough to require that $\mathbf{b}(s)$ is generated by a Rellich potential. To satisfy condition (3.1) we must also require that the *a priori* probability density $\pi(\gamma')$ is such that

$$E\left[\int_0^t ds\, \mathbf{b}(s)^2\right] = \int_0^t ds \int d\pi(\gamma') E'[\mathbf{b}[\mathbf{x}(s),\gamma',s]^2] < \infty. \tag{6.1}$$

Notice that for Rellich potentials it is true that the integral over time in (6.1) exists, but this does not imply that the integral over the measure $d\pi(\gamma')$ is necessarily finite. It is interesting to see that if the drift terms $\mathbf{b}(s)$ are generated by Rellich potentials for every choice of γ we have that condition (5.1) holds so the Rao–Cramer matrix introduced in Sec. V can be constructed.

By analogy it may be expected that the solution (4.11) to the Kushner equation (3.4) provides an explicit form for the *a posteriori* probability density of the parameters γ in (2.4a), but it is not easy to apply the theorem since its condi-

tions are difficult to check.[11] Nonetheless, the next theorem shows that to obtain an *a posteriori* density similar to (4.11) no more is required than that the drift term in (2.4b) be generated by a Rellich potential for very γ and that $\pi(\gamma')$ is such that (6.1) holds. For the proof of the theorem we will make use of the extended Bayes formula.[11]

Theorem VI.2: We assume that the drift $\mathbf{b}(s)=\mathbf{b}[x,\gamma',s]$ is generated by a Rellich potential for all $\gamma'\in R^K$ and that the *a priori* density is such that (6.1) holds. In addition, let the drift depend continuously on γ' and let $F_s^{\mathbf{r}}$ be the minimal sigma algebra containing all the sigma algebras associated with the solutions to (2.4b) for all γ'. Then we have that for any function g: $R^K\to R$, with $E[g(\gamma')]=\int d\pi(\gamma')g(\gamma')<\infty$,

$$E\left[g(\gamma')|F_s^{\mathbf{r}}\right]=\int_{R^K}d\pi(\gamma')g(\gamma',\mathbf{x})\rho(\gamma',\mathbf{r}), \tag{6.2}$$

where

$$\rho(\gamma',\mathbf{r})=\exp\left[\frac{1}{\sigma^2}\Gamma_s(\mathbf{b}(s))-\frac{1}{2\sigma^2}\int_0^s d\tau\,\mathbf{b}(\tau)^T\cdot\mathbf{b}(\tau)\right]\times\left\{\int_{R^K}d\pi(\gamma')\exp\left[\frac{1}{\sigma^2}\Gamma_s(\mathbf{b}(s))-\frac{1}{2\sigma^2}\int_0^s d\tau\,\mathbf{b}(\tau)^T\cdot\mathbf{b}(\tau)\right]\right\}^{-1} \tag{6.3}$$

on $[0,t]$, where $\Gamma_s(\mathbf{b}(s))=\Gamma_s(\mathbf{b}[\mathbf{r}(s),\gamma',s])$ is defined in (5.4) and (5.5).

Let $d\eta(s)=\sigma\,d\mathbf{w}(s)$, $0\leqslant s\leqslant t$, for the Wiener process $\mathbf{w}(s)$ in (2.4b) and let μ_η be the measure associated with $\eta(s)$ and $\mu_{\mathbf{x}(\gamma')}$ be the measure associated with the stochastic process that is the solution to (2.4b) for the drift $\mathbf{b}[x(s),\gamma',s]$. If it is true that

$$p\left[\int_0^t d\tau[\mathbf{b}[\eta(\tau),\gamma',\tau]]^2<\infty\right]=1 \tag{6.4}$$

for all γ' so that $\mu_{\mathbf{x}(\gamma')}\sim\mu_\eta$ (see Ref. 11) for all γ', then (6.2) holds with the function $\rho(\gamma',\mathbf{r})$:

$$\rho(\gamma',\mathbf{r})=\exp\left[\frac{1}{\sigma^2}\int_0^s\mathbf{b}(\tau)^T\cdot d\mathbf{r}(\tau)-\frac{1}{2\sigma^2}\int_0^s d\tau\,\mathbf{b}(\tau)^T\cdot\mathbf{b}(\tau)\right]\times\left\{\int_{R^K}d\pi(\gamma')\exp\left[\frac{1}{\sigma^2}\int_0^s\mathbf{b}(\tau)^T\cdot d\mathbf{r}(\tau)-\frac{1}{2\sigma^2}\int_0^s d\tau\,\mathbf{b}(\tau)^T\cdot\mathbf{b}(\tau)\right]\right\}^{-1} \tag{6.5}$$

with $\mathbf{b}(\tau)=b[\mathbf{r}(\tau),\gamma',\tau]$.

Proof: Let $\mathbf{x}(\gamma',s)$ be the solution to (2.4b) for a given vector $\gamma'\in R^K$, and let $\mathbf{x}(\gamma')=\{\mathbf{x}(\gamma',s')\}_{0\leqslant s'\leqslant s}$. The process $\mathbf{x}(\gamma',s)$ has a continuous version because it is a square integrable martingale. Let $\mu_{\mathbf{x}(\gamma')}$ and $F_s^{\mathbf{x}(\gamma')}$ be the measure and sigma algebra associated with the process $\mathbf{x}(\gamma')$ and let $d\eta(s')=\sigma\,d\mathbf{w}(s')$, $0\leqslant s'\leqslant s$, with $\sigma^2=\hbar/m$, where $\mathbf{w}(s)$ is the standard Wiener process in (2.4b). The continuity of $\mathbf{x}(\gamma',s)$ also implies that $F_s^{\mathbf{x}(\gamma')}$ is a separable sigma algebra. Denote the minimal sigma algebra that contains all the sigma algebras $F_s^{\mathbf{x}(\gamma')}$ by $F_s^{\mathbf{r}}$ and assume that it is complete. Because the drift is continuous in γ' and because all algebras $F_s^{\mathbf{x}(\gamma')}$ are separable, we find that the $F_s^{\mathbf{r}}$ is also separable.

Consider the combined process $(\gamma',\mathbf{x}(\gamma',s'))$. The outcome space of the combined process is $R^K\times C[0,s]^N$, where $C[0,s]^N$ is the collection of N-dimensional continuous functions on $[0,s]$, and the minimal sigma algebra associated with this outcome space is given by $F(R^K)\times F_s^{\mathbf{r}}$, where $F(R^K)$ is the Borel algebra of R^K and $F_s^{\mathbf{r}}$, which is the sigma algebra associated with the collection of stochastic processes $\mathbf{x}(\gamma',s)$. Also, $F(R^K)\times F_s^{\mathbf{r}}$ is the minimal sigma algebra containing all sets $A\times B$, $A\in F(R^K)$ and $B\in F_s^{\mathbf{r}}$, which is assumed to be complete. The sigma algebra $F(R^K)\times F_s^{\mathbf{r}}$ is separable because $F(R^K)$ and $F_s^{\mathbf{r}}$ are separable. The measure $\mu_{\gamma\mathbf{r}}$ on the algebra is determined if it is defined on all sets $A\times B$, since its extension to the whole sigma algebra $F(R^K)\times F_s^{\mathbf{r}}$ is now unambiguous. Let $A\times B\in F(R^K)\times F_s^{\mathbf{r}}$, then we may define

$$\mu_{\gamma\mathbf{r}}(A\times B)=\int_{\gamma'\in A}d\pi(\gamma')P(\mathbf{x}(\gamma')\in B)=\int_{\gamma'\in A}d\pi(\gamma')\int_{\mathbf{r}\in B}d\mu_{\mathbf{x}(\gamma')}(\mathbf{r}), \tag{6.6}$$

where the measure $\pi(\gamma')$ is the initial probability density for the parameters $\gamma_1,\ldots,\gamma_K$. Since for any value of γ' the stochastic process $\mathbf{x}(\gamma',s)$ is associated with a Rellich potential we see that (6.1) holds for any $\mathbf{b}[\mathbf{x}(\gamma',s),\gamma',s]$. Hence

$$p\left[\int_0^t d\tau\,b[\mathbf{x}(\gamma',\tau),\gamma',\tau]^2<\infty\right]=1 \tag{6.7}$$

for all γ', which implies that $\mu_{\mathbf{x}(\gamma')}\ll\mu_\eta$. Equation (6.7) can then be written as

$$\mu_{\gamma\mathbf{r}}(A\times B)=\int_{\gamma'\in A}d\pi(\gamma')\int_{\mathbf{r}\in B}d\mu_\eta(\mathbf{r})\frac{d\mu_{\mathbf{x}(\gamma')}}{d\mu_\eta}(\mathbf{r},s) \tag{6.8}$$

using the Radon–Nikodym derivative (5.2) [replacing $\mathbf{x}$ by $\mathbf{x}(\gamma')$].

From (6.8) we see that the conditional probability density $Q[B,\gamma']$ is given by

$$Q[B,\gamma']=\int_{\mathbf{r}\in B}d\mu_\eta(\mathbf{r})\frac{d\mu_{x(\gamma')}}{d\mu_\eta}(\mathbf{r},s). \tag{6.9}$$

By construction this conditional probability density is regular and from (6.9) follows that for all $\gamma'\in R^K$, $Q[\cdot,\gamma']\ll\mu_\eta$. Applying Lemma 7.4 in Ref. 10 we obtain

$$E\left[g(\gamma')|F_s^{\mathbf{r}}\right]=\left(\int_{R^K}d\pi(\gamma')g(\gamma')\frac{d\mu_{x(\gamma')}}{d\mu_\eta}(\mathbf{r},s)\right)\times\left(\int_{R^K}d\pi(\gamma')\frac{d\mu_x(\gamma')}{d\mu_\eta}(\mathbf{r},s)\right)^{-1}, \tag{6.10}$$

where the Radon–Nikodym derivative is given by (5.2) with $\mathbf{b}(s)=\mathbf{b}[\mathbf{r}(s),\gamma',s]$. The function $\Gamma_s(\mathbf{b}(s))$ is again defined by (5.4) and (5.5) so (6.10) now establishes (6.3).

If, in addition, (6.4) holds then $\mu_{\mathbf{x}(\gamma')}\sim\mu_\eta$ so that the function $\Gamma_s(\mathbf{b}(s))$ assumes the form of the integral over its argument, which reduces (6.3) to (6.5). Q.E.D.

VII. CONCLUSIONS

In this paper we assumed that the experimental observations on quantal systems can be represented as a realization of the random variable $\mathbf{x}(s)$ associated with the probability density $|\psi[x,s]|^2$, where the wave function ψ satisfies the Schrödinger equation. Using stochastic mechanics and some results from filtering theory, we established by simple examples that a realization of this random variable over a continuous period of time can be effectively used to estimate the unknown initial momentum for a free particle or the unknown parameters in a harmonic potential. In the more general case that the potential in the Schrödinger equation is a Rellich potential for all the possible values of the unknown (time independent) parameters, an optimal estimator for the unknown parameter can be constructed if the initial estimated average energy is finite. We explicitly calculated the analytical form of the *a posteriori* probability density of the parameters in this case using the extended Bayes formula. If the state of the system (2.5a) is nondeterministic, the *a posteriori* probability distribution is difficult to construct and the Kushner equation is then only analytically soluble if the potential is of the type $V = ax^2 + bx + c$ with appropriate initial conditions.[17]

It would be especially interesting to extend the estimation procedure to scattering phenomena, where only the initial and final realizations of the stochastic processes can be observed. Filtering techniques have been developed for the case that the observations can only be measured on a restricted interval and this can be applied to scattering problems. Unfortunately the asymptotic properties of processes described by stochastic mechanics are not well understood (for some results in this direction see Refs. 5, 8, and 18) and some of the notions in scattering theory (for instance, the S matrix) do not translate easily to stochastic processes.

One of the approximations that has been developed in the context of filtering theory is especially useful for the parameter estimation problem formulated in this paper. The inversion of the observational data from (2.4a) and (2.5b) depends on the variance σ. Since this constant is small (it is proportional to $\hbar/m$) the behavior of the estimator in the asymptotic limit $\sigma \to 0$ becomes of interest. This small noise approximation is rather well developed in the system literature,[9,19,20] and consequently can be fruitfully applied to parameter estimation in quantal systems.

The proof of Theorem 6.2 in Sec. VI suggests an extension to the countably infinite dimensional case where the entire potential is unknown. The state and observational equations then assume the form of the functional analog to (2.5a) ($\delta V(x) = 0$), where the drift simply depends on the potential $\mathbf{b}(s) = \mathbf{b}[\mathbf{x}(s),V,s]$. It is necessary to specify in what space the potential exists and in view of our previous discussion, it would be natural to search for a potential of the Rellich type. In R^3 the space of such potentials is well known to be $L^2 + L^\infty$, i.e., any Rellich potential in R^3 can be written as the sum of a function in $L^2 = \{f | \int dx\, f^2 < \infty\}$ and a function in $L^\infty = \{f | \sup_x |f| < \infty\}$. To reproduce the Bayesian argument of Theorem 6.2 for the finite dimensional case, we have to determine a sigma algebra on the space of Rellich potentials to take the place of the Borel algebra $F(R^K)$ in Theorem 6.2. The *a posteriori* probability distribution changes into a measure on the space of Rellich potentials conditional on the sigma algebra $F_s^{\mathbf{x}(V)}$ [i.e., the collection of events generated by $\mathbf{x}(V,s')$, $0 \leqslant s' \leqslant s$, for all $V \in L^2 + L^\infty$]. By analogy to Sec. VI, the conditional measure $\mu[V|F_s^r]$ [F_s^r is now the sigma algebra of events $\mathbf{x}(V) = \{\mathbf{x}(V,s')\}_{0<s'<s}$, $V \in L^2 + L^\infty$], can be symbolically written as

$$d\mu[V|F_s^r] = \exp\left[\Gamma_s(b[\mathbf{r}(s),V,s]) - \frac{1}{2}\int_0^s b^2[V,\mathbf{r}(\tau),\tau]d\tau\right]d\mu[V] \times\left\{\int_{L^2+L_\infty}\exp\left[\Gamma_s(b[\mathbf{r}(s),V,s]) - \frac{1}{2}\int_0^s b^2[V,\mathbf{r}(\tau),\tau]d\tau\right]d\mu[V]\right\}^{-1}, \quad (7.1)$$

where $d\mu[V]$ is the *a priori* probability distribution for V and where $\Gamma_s(\mathbf{b}(s))$ is defined in (5.3) and (5.4) with $\mathbf{b}(s) = \mathbf{b}[\mathbf{r}(s),V,s]$. This expression is Bayesian in nature and provides the *a posteriori* probability measure for the functional state, conditional on a realization $\{\mathbf{r}(s')\}_{0<s'<s}$. We leave more formal investigations along these lines to future research.

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An application of filtering theory to parameter identification in quantum mechanics

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A method for inverting observations on quantum mechanical systems to obtain estimates of unknown parameters residing in the Hamiltonian is presented. The quantal system is represented in matrix form with respect to a chosen basis, and it is assumed that the associated expansion coefficients are truncated to a finite dimension. The uncontrollable laboratory noise will be modeled by means of an inhomogeneous white noise process so that the experimental observations are represented as stochastic variables satisfying a stochastic differential equation. It will be assumed that measurements obtained from an experiment are now equivalent to a realization of these stochastic variables. It is known from filtering theory that the minimum variance estimate of the unknown parameters in the quantal model is now given by the expectation of the unknowns conditional on this realization. This estimator can be calculated analytically from the associated *a posteriori* probability density if the original quantal system does not contain any random elements. This probability density for the unknown matrix elements is calculated, and it is demonstrated that for a full Hamiltonian matrix the asymptotic variance of the parameter estimator decreases as a third power in time and a fourth power in the initial conditions. Some differences with the minimum least-square method are mentioned, and a few issues of numerical implementation are discussed.

I. INTRODUCTION

Many problems in physics and chemistry require inverting experimental data in order to obtain estimates of unknown potentials. Most rigorous approaches to inversion problems are based on the analytical properties of the wave function. These methods effectively assume that the wave function is a measurable quantity, which is not the case since the wave function determines the amplitude of the particles but is not itself an observable. Using filtering theory we develop a new approach for inverting experimental data that explicitly allows for the observables to be quadratic forms of the wave function, thereby encompassing true measurables.

Our method is based on a combination of matrix mechanics, introduced in Sec. II, and filtering theory, presented in Sec. III. Briefly, the time-dependent wave function is first expanded in the usual fashion with respect to an appropriate basis. The resulting expansion coefficients satisfy a set of linear differential equations and depend on unknown initial conditions and unknown parameters residing in the Hamiltonian matrix. The set of equations for the quantal system is usually infinite, but we consider only a finite subset in keeping with most practical procedures for solution. The experimental measurements are proportional to the weighted quadratic combinations of the expansion coefficients and are often influenced by additional physical processes that are not explicitly included in the model. These extraneous effects may be modeled by means of an additive white noise process so that the experimental observations become a stochastic variable. Our assumption will be that a particular measurement on the quantal system is given by a realization of this stochastic variable.

It is well known in filtering theory that the minimum variance estimator for the unknown parameters and initial conditions from the available information is given by the *a posteriori* mean of the unknown quantities conditional on this realization.[1-4] The optimal estimate, also referred to as a filter, satisfies a stochastic integral equation[3-5] and the *a posteriori* probability distribution necessary to calculate the conditional mean satisfies a stochastic partial differential equation known as the Kushner equation.[1-7] The latter equation can be solved analytically if the equations for the quantal system are entirely deterministic.

Under appropriate circumstances, the covariance matrix of an estimator asymptotically approaches the inverse of the Rao–Cramer lower bound introduced in Sec. III.[1,4] We show that if the equation for the expansion coefficients is deterministic this matrix can be obtained from the sensitivity equations of the quantal model. In Sec. IV the filtering method is used to construct the estimator for the unknown parameters in the Hamiltonian matrix and we obtain information on the asymptotic variance of this estimator from the associated Rao–Cramer lower bound matrix. Finally, in Sec. V the paper is summarized and the conclusions are presented.

This approach is different from the parameter estimation method developed in Ref. 8 using stochastic mechanics, though both approaches use filtering methods. Here we assumed that the measurement is proportional to the quantum mechanical expectation and an inhomogeneous white noise process modeling the experimental error. If the variance of

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this stochastic process approaches zero the observation will reduce to the quantum mechanical expectation, which is not the case in Ref. 8. There the only source of error was the noise term prescribed by stochastic mechanics with a variance proportional to Planck's constant. If that inhomogeneous noise term were to vanish, the observations would reduce to exact measurements on a Newtonian system. The various expressions in these two papers must therefore carry a different interpretation.

Section II introduces the assumptions on the quantal system and the experimental observations that allow the estimation of the residing unknown parameters to be represented as a filtering problem.

II. THE QUANTUM MECHANICAL SYSTEM

The quantal system will be represented in matrix form where the expansion vector $\mathbf{v}(s)$ is truncated to the finite dimension L, while the experimental observations are assumed to satisfy a stochastic differential equation. The unknown parameters in the Hamiltonian matrix and the initial conditions for the expansion coefficients must then be estimated from a realization of this stochastic variable. The method below can be generalized to infinite dimensional systems, but the estimation problem is more manageable if the basis set is finite.

Hence the expansion vector $\mathbf{v}(s)\,R^L$ satisfies the following equation:

$$i\hbar\frac{d}{ds}\mathbf{v}(s)=\mathsf{H}\mathbf{v}(s)\,, \tag{2.1}$$

where elements of the vector $\mathbf{v}(s)$ are the projection of the wave function ψ, $(\mathbf{v})_i=\langle\phi_i|\psi\rangle$, $i=1,...,L$, with ϕ_j, $j=1,...,L$, being members of an orthonormal basis set. The Hamiltonian matrix H is related to the operator $\hat{H}$ via $(\mathsf{H})_{ij}=\langle\phi_i|\hat{H}|\phi_j\rangle$, $i,j=1,...,L$. At best only limited information is assumed to be available on the potential, therefore some or all of the matrix elements of the matrix H are unknown. The Hamiltonian matrix includes all relevant physical effects, except those arising due to uncontrollable laboratory measurement processes.

We further assume that the observations $\mathbf{z}(s)\in R^M$ on the system with the variables $\mathbf{v}(s)$ are given by the usual sum of the weighted squares of the expansion coefficients $v_1(s),...,v_L(s)$ plus laboratory noise that has been modeled by means of a Wiener process. The random terms incorporate all the physical processes that influence the experimental observations $\mathbf{z}(s)$ which are not included in the model (2.1). As a result of this assumption the experimental observations $\mathbf{z}(s)$ satisfy an M dimensional stochastic differential equation

$$d\mathbf{z}(s)=\mathbf{G}(s)ds+\mathsf{P}\,d\mathbf{w}_1(s)\,, \tag{2.2}$$

where $(\mathbf{G}(s))_k=\Sigma_{i,j=1}^{L}\left[O_{kij}v_i(s)v_j^*(s)\right]$, $k=1,...,M$, with $\mathbf{w}_1(s)$ being an M dimensional Wiener process. The matrix elements O_{kij}, $i,j=1,...,L$, $k=1,...,M$, prescribe the relation between the k th observation and elements of the vector $\mathbf{v}(s)$, while elements of the matrix P indicate the magnitude of the stochastic fluctuations. Typically, the matrices O_{kij} are symmetric in the indices i and j for all $k=1,...,M$, so that the function $\mathbf{G}(s)$ in (2.2) is real (this is the case assumed here).

The unknowns in the system are the initial conditions of the expansion coefficients $\mathbf{v}(0)$ in (2.1) and a vector of unknown parameters $\alpha=(\alpha_1,...,\alpha_K)$ in the Hamiltonian matrix. Casting Eq. (2.1) in terms of real variables, writing $\mathbf{v}(s)=\mathbf{v}(s)^{(1)}+i\mathbf{v}(s)^{(2)}$, $\mathbf{v}(s)^{(1)}\in R^L$, $\mathbf{v}(s)^{(2)}\in R^L$, and defining $\mathbf{v}'(s)^T=(\mathbf{v}(s)^{(1)T},\mathbf{v}(s)^{(2)T},\alpha^T)$, the vector $\mathbf{v}'(s)$ can be easily shown to satisfy

$$\frac{d}{ds}\mathbf{v}'(s)=\mathsf{H}'(\alpha)\mathbf{v}'(s)=\mathsf{H}'(\mathbf{v}'(s))\mathbf{v}'(s)\,, \tag{2.3}$$

where

$$\mathsf{H}'(\alpha)=\frac{1}{\hbar}\begin{bmatrix}0 & \mathsf{H}(\alpha) & 0\\ -\mathsf{H}(\alpha) & 0 & 0\\ 0 & 0 & 0\end{bmatrix}. \tag{2.4}$$

Notice that the matrix H' only depends on the last K variables of $\mathbf{v}'(s)$, which coincide with the parameters. Equations (2.3) and (2.2) are usually referred to as state and observational equations, where $\mathbf{v}'(s)$ is the unknown state and where $\mathbf{z}(s)$ incorporates the observational data. The main assumption of our paper is that an experimental observation on the quantal system over a time s is equivalent to a realization of the random variables $\mathbf{z}(s')$ on the interval $[0,s]$ and an application of the filtering methods below will yield an estimate for the initial conditions of the state $\mathbf{v}'(0)=\theta$ given this realization. As a result, this procedure yields an estimator for all initial conditions $\theta_1,...,\theta_{2L}$ and the unknown parameters $\theta_{2L+1},...,\theta_{2L+K}$ in the Hamiltonian matrix.

It is possible that the state $\mathbf{v}'(s)$ in (2.3) is influenced by additional physical processes that affect the potential in the Hamiltonian matrix H or influence the vector $\mathbf{v}(s)$ in (2.1) (e.g., the system could be subject to external fluctuations, etc.). These processes are not part of the nominal equations, and in an effort to model this we assume that Eq. (2.3) is perturbed by another Wiener process $\mathbf{w}_2(s)$. In that case, the state and observational equations (2.3) and (2.2) change into the following stochastic differential equations:

$$d\mathbf{v}'(s)=\mathsf{H}'(\mathbf{v}'(s))\mathbf{v}'(s)ds+\mathsf{Q}(\mathbf{v}'(s))d\mathbf{w}_2(s)\,, \tag{2.5a}$$

$$d\mathbf{z}(s)=\mathbf{G}(s)ds+\mathsf{P}\,d\mathbf{w}_1(s)\,, \tag{2.5b}$$

where $\mathbf{w}_1(s)$ and $\mathbf{w}_2(s)$ are independent Wiener processes of appropriate dimension. The magnitude of the fluctuations that perturb the state $\mathbf{v}'(s)$ is given by the matrix Q, which in most physical cases depends on the expansion coefficients. For instance, if the potential contains random elements, Q depends linearly on the state $\mathbf{v}'(s)$.

Section III briefly summarizes the basic filtering theorems necessary to find an estimator for the unknown initial condition $\mathbf{v}'(0)$ given a realization of the stochastic variable $\mathbf{z}(s)$ satisfying (2.5b).

III. STOCHASTIC FILTERING THEORY

It is well known from filtering theory that the minimum variance estimate of the state $\mathbf{v}'(0)$ in (2.5a) given the realization $A_s=\{\mathbf{z}(s)\}_{0<s'<s}$, where $\mathbf{z}(s)$ satisfies (2.5b), is equivalent to the mean of $\mathbf{v}'(0)$ conditional on the realization A_s.[3,4] The *a posteriori* probability density necessary to calculate the optimal estimator satisfies a stochastic partial

differential equation known as the Kushner equation, which can be easily solved if the state equation (2.5a) does not contain noise (i.e., if $\mathsf{Q}=\mathbf{0}$).[1,4] We also introduce the Rao–Cramer lower bound matrix, which will be used to describe the asymptotic behavior of the covariance matrix of this parameter estimator. If Eq. (2.5a) is deterministic, the Rao–Cramer matrix can be obtained from the sensitivity equations of (2.1).

The optimal estimator for the initial conditions $\mathbf{v}'(0)$ given the realization $A_s=\{\mathbf{z}(s)\}_{0\leqslant s'\leqslant s}$ is the functional $\mathbf{\Phi}_s$ of A_s that minimizes the variance of the difference $\Delta=\mathrm{Tr}\,E[(\mathbf{v}'(0)-\mathbf{\Psi}_s)(\mathbf{v}'(0)-\mathbf{\Psi}_s)^T]$ and is given by $\mathbf{\Phi}_s=E[\mathbf{v}'(0)|A_s]$.[1–4] Here Tr denotes the matrix trace operation and E is the expectation over all random processes. The estimator is often referred to as a filter and may be expressed as $\mathbf{\Phi}_s=\int d\mathbf{x}\,\mathbf{x}\rho[\mathbf{x}|A_s]$, where $\rho[\mathbf{x}|A_s]$ is the *a posteriori* probability density of the state $\mathbf{v}(0)$ conditional on the realization A_s. Under the reasonable condition

$$\int_0^t ds\,E[\mathbf{F}(s)^2]<\infty,\quad \int_0^t ds\,E[\mathbf{G}(s)^2]<\infty, \tag{3.1}$$

and some additional requirements on the drift functions, it can be shown[1,2,4,7] that the density $\rho[\mathbf{x}|A_s]$ satisfies the Kushner equation

$$\begin{aligned} d\rho[\mathbf{x}|A_s] &= \rho[\mathbf{x}|A_s][(\mathbf{G}(s)-E[\mathbf{G}(s)|A_s])^T\mathsf{U}^{-1}(d\mathbf{z}(s) \\ &\quad -E[\mathbf{G}(s)|A_s]ds)], \end{aligned} \tag{3.2}$$

where $\mathsf{U}=\mathsf{P}\mathsf{P}^T$. This equation has to be interpreted in the sense of Ito and contains implicit terms like $E[\mathbf{G}(s)|A_s]$.

There are a number of occasions in which the solution for (3.2) can be obtained analytically. For instance, if the functions $\mathbf{G}(s)$ and $\mathbf{F}(s)$ in (2.5a) are, respectively, linear in the variables $\mathbf{v}'(s)$ and $\mathbf{z}(s)$, an explicit solution for the estimator can be found.[3,4,7,9] Equation (3.2) can also be solved if the matrix Q in (2.5a) becomes zero. In that case the *a posteriori* probability density for the state $\mathbf{v}'(0)=\boldsymbol{\theta}$ given the realization A_s from the solution to Eq. (2.5b) is given by

$$\rho[\mathbf{x}|A_s]=\frac{q_s[\mathbf{x}]}{\int d\mathbf{x}\,q_s[\mathbf{x}]}, \tag{3.3}$$

where $q_s[\mathbf{x}]$ satisfies the equation $dq_s[\mathbf{x}]=q_s[\mathbf{x}]\mathbf{G}(s)^T\mathsf{U}^{-1}\,d\mathbf{z}(s)$ and is usually referred to as the unnormalized probability function.[1,4] The initial condition for this equation, $q_0[\mathbf{x}]$, is the probability density containing the initial information on the parameters $\boldsymbol{\theta}$. Solving the equation for the unnormalized density yields

$$\begin{aligned} q_s[\mathbf{x}] &= q_s[\mathbf{X}(0)]\exp\left[\int_0^s -\frac{1}{2}(\mathbf{G}(\tau))^T\mathsf{U}^{-1}\mathbf{G}(\tau)d\tau\right. \\ &\quad \left.+(\mathbf{G}(\tau))^T U^{-1}d\mathbf{z}(\tau)\right], \end{aligned}$$

where

$$\frac{d\mathbf{X}(\tau)}{d\tau}=\mathbf{H}'[\mathbf{X}(\tau)], \tag{3.4}$$

$\mathbf{G}(s)=\mathbf{G}[\mathbf{X}(s)]$ with the final conditions $\mathbf{X}(s)=\mathbf{x}$. The integral must be evaluated in the sense of Stratonovich.

The Rao–Cramer inequality yields a lower bound that gives information on the asymptotic behavior of the covariance matrix of an estimator[1,4] and can be found as follows. Let $d\boldsymbol{\eta}(s)=\mathsf{P}\,d\mathbf{w}_1(s)$ and assume that μ_η and μ_z are the respective measures of the stochastic processes $\boldsymbol{\eta}(s)$ and $\mathbf{z}(s)$. The latter process depends on $\boldsymbol{\theta}$ via the observational function $\mathbf{G}(s)$. Consequently, the Radon–Nikodym derivative[4] of the measure μ_z, with respect to the measure μ_η, also depends on $\boldsymbol{\theta}$ and will be denoted $\Gamma(s,\boldsymbol{\theta})$. Its existence is assured by (3.1).[4] Consequently, the set of functionals ν_j, $j=1,\ldots,2L+K$,

$$\nu_j=\frac{\partial}{\partial\theta_j}\{\log\Gamma(s,\boldsymbol{\theta})\}, \tag{3.5}$$

is well defined and has a covariance matrix $\mathsf{Z}=E'[\boldsymbol{\nu}\boldsymbol{\nu}^T]$, where the expectation E' is solely over the stochastic variable $\{\mathbf{z}(s')\}_{0\leqslant s'\leqslant s}$ (the matrix Z therefore depends on $\boldsymbol{\theta}$). Let $\mathsf{A}=E'[\boldsymbol{\phi}\boldsymbol{\nu}^T]-E[\boldsymbol{\phi}^T]E'[\boldsymbol{\nu}^T]=E'[\boldsymbol{\phi}\boldsymbol{\nu}^T]$; then, for any estimator $\boldsymbol{\phi}_s$: $\{\mathbf{z}(s')\}_{0\leqslant s'\leqslant s}\to R^{2L+K}$ of the parameter vector $\boldsymbol{\theta}$ with covariance matrix $\mathsf{R}=E[\boldsymbol{\phi}\boldsymbol{\phi}^T]-E[\boldsymbol{\phi}]E[\boldsymbol{\phi}]^T$, we have that the matrix combination $\mathsf{R}-\mathsf{A}(\mathsf{Z})^{-1}\mathsf{A}^T$ is positive definite or $\mathsf{R}-\mathsf{A}(\mathsf{Z})^{-1}\mathsf{A}^T\geqslant 0$. From this point on we shall assume that under the present conditions as time increases to infinity, the estimators become unbiased ($\mathsf{A}\to\mathsf{I}$) and the covariance matrix R asymptotically approaches the inverse of the Rao–Cramer lower bound matrix Z^{-1}. Some of the conditions necessary for this asymptotic behavior are known[1,4,8] but more work on the general case still needs to be done. For the proof of this version of the Rao–Cramer bound see Ref. 8.

There is an interesting consequence of this inequality. If Eq. (2.5a) is deterministic, i.e., if $\mathsf{Q}=\mathbf{0}$ then the Rao–Cramer lower bound for the estimator of the initial conditions reduces to

$$\begin{aligned} (\mathsf{Z})_{pk} &= \sum_{a,b=1}^{M} U_{ab}^{-1}\int_0^s ds'\,\frac{\partial G_a(s')}{\partial\theta_p}\frac{\partial G_b(s')}{\partial\theta_k} \\ &= \sum_{a,b=1}^{M} U_{ab}^{-1}\int_0^s ds'\sum_{p,k=1}^{J}\frac{\partial G_a(s')}{\partial v_p'} \\ &\quad\times\frac{\partial G_b(s')}{\partial v_k'}\frac{\partial v_p}{\partial\theta_p}\frac{\partial v_k}{\partial\theta_k}, \end{aligned} \tag{3.6}$$

where U^{-1} is the inverse of the matrix $\mathsf{U}=\mathsf{P}^T\mathsf{P}$. The partial derivatives of the expansion coefficients with respect to $\boldsymbol{\theta}$ can be obtained from the sensitivity equations of (2.1).

Section IV uses the filter and the Rao–Cramer lower bound matrix to find analytical information on the estimator of the initial conditions and unknown parameters in a deterministic quantal model.

IV. APPLICATIONS AND EXAMPLES

Using (3.3) and (3.4) we can derive the analytical form for the estimator of the parameters $\mathbf{v}'(0)=\boldsymbol{\theta}$ in (2.5a) given a realization $\{\mathbf{z}(s)\}_{0\leqslant s'\leqslant s}$, where $\mathbf{z}(s)$ is the observational vector defined in (2.5b). We obtain the estimator in the case that the time-independent Hamiltonian matrix is diagonal and we calculate the Rao–Cramer lower bound matrix for the full Hamiltonian.

Let $\mathsf{P}=\gamma\mathsf{I}$ and partition the vector $\mathbf{X}(s)=(\mathbf{X}_1(s),\mathbf{X}_2(s),\mathbf{X}_3(s))$, $\mathbf{X}_1(s),\mathbf{X}_2(s)\in R^L$, and $\mathbf{X}_3(s)\in R^K$. Substitut-

ing the observational function $G(s)$ into the expression for the unnormalized probability density, we find that

$$q_s[\mathbf{x}] = q_0[\mathbf{X}(0)]\exp\left[-\frac{1}{2\gamma^2}\sum_{k=1}^{M}\left[\sum_{i,j=1}^{L} O_{kij}\left[(\mathbf{X}_1(\tau))_i(\mathbf{X}_1(\tau))_j + (\mathbf{X}_2(\tau))_i(\mathbf{X}_2(\tau))_j\right]\right]^2 d\tau\right.$$
$$\left.+\frac{1}{\gamma^2}\sum_{k=1}^{M}\left[\sum_{i,j=1}^{L} O_{kij}\left[(\mathbf{X}_1(\tau))_i(\mathbf{X}_1(\tau))_j + (\mathbf{X}_2(\tau))_i(\mathbf{X}_2(\tau))_j\right]dz_k(\tau)\right]\right], \tag{4.1}$$

where

$$\frac{d}{d\tau}\mathbf{X}(\tau) = \mathsf{H}'(\mathbf{X}(\tau))\mathbf{X}(\tau) = \mathsf{H}'(\mathbf{X}_3(\tau))\mathbf{X}(\tau), \tag{4.2}$$

with the final conditions $\mathbf{X}(s) = (\mathbf{X}_1(s),\mathbf{X}_2(s),\mathbf{X}_3(s)) = (\mathbf{x}_1,\mathbf{x}_2,\mathbf{x}_3) = \mathbf{x}$, $\mathbf{x}_1,\mathbf{x}_2 \in R^L$, and $\mathbf{x}_3 \in R^K$. Here $q_0[\mathbf{x}]$ is the initial probability density.

Equation (4.2) can be solved to yield

$$\mathbf{X}(\tau) = \begin{bmatrix} \cos[\mathsf{H}(\mathbf{x}^{(3)})(\tau-s)/\hbar] & \sin[\mathsf{H}(\mathbf{x}^{(3)})(\tau-s)/\hbar] & \mathbf{0} \\ -\sin[\mathsf{H}(\mathbf{x}^{(3)})(\tau-s)/\hbar] & \cos[\mathsf{H}(\mathbf{x}^{(3)})(\tau-s)/\hbar] & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathsf{I} \end{bmatrix}\begin{bmatrix}\mathbf{x}_1\\ \mathbf{x}_2\\ \mathbf{x}_3\end{bmatrix}, \tag{4.3}$$

which determines the functions $\mathbf{X}_1(\tau)$, $\mathbf{X}_2(\tau)$, and $\mathbf{X}_3(\tau)$ in (4.1). The *a posteriori* distribution for θ, $\rho[\mathbf{x}|A_s]$, $\mathbf{x}\in R^{2L+K}$, conditional on the realization $A_s = \{\mathbf{z}(s')\}_{0<s'<s}$, can subsequently be obtained from (4.1) and (3.3). The construction shows that the probability density $q_s[\mathbf{x}]$ must be evaluated for every point $\mathbf{x}\in R^{2L+K}$, which means that the characteristic functions $\mathbf{X}_1(\tau)$ and $\mathbf{X}_2(\tau)$ have to be calculated for every final condition $\mathbf{x}$. If the Hamiltonian matrix contains many expansion coefficients or many unknown parameters so that K or L become large, then a large amount of computer memory will be required. To reduce the necessary parameter space, it is possible to derive the marginal distribution for the unknown parameters in the Hamiltonian matrix by integrating $\rho[x|A_s]$ over the first two sets of variables and normalizing the resulting distribution with respect to the remaining variables $\mathbf{x}^{(3)}$. In most applications the number of parameters in the potential is usually small.

If the noise term in the state $\mathbf{v}'(s)$ in (2.5a) is nonzero, a simple solution such as the one above cannot be readily obtained, but many analytical results for estimation on a noisy state can be found in Refs. 1, 4, 9, and 10. In addition, many numerical algorithms and approximations have been developed for this case and can be brought to bear on the estimation problem above.

As an example, let us assume that H is a diagonal matrix, $\mathsf{H} = \Lambda$, where $(\Lambda)_{ij} = \delta_{ij}\alpha_j$, $i,j = 1,...,L$, so that the unknown parameters are the diagonal matrix elements α_j, $j = 1,...,L$, and the $2L$ initial conditions $v(0)^{(1)}$, $\mathbf{v}(0)^{(2)}$. From (4.3) we see that the functions $\mathbf{X}_1(\tau)$, $\mathbf{X}_2(\tau)$, and $\mathbf{X}_3(\tau)$ become

$$(\mathbf{X}_1(\tau))_j = \cos[x_j^{(3)}(\tau-s)/\hbar]\cdot x_j^{(1)} + \sin[x_j^{(3)}(\tau-s)/\hbar]\cdot x_j^{(2)},$$
$$(\mathbf{X}_2(\tau))_j = -\sin[x_j^{(3)}(\tau-s)/\hbar]\cdot x_j^{(1)} + \cos[x_j^{(3)}(\tau-s)/\hbar]\cdot x_j^{(2)},$$
$$\mathbf{x}_3(\tau) = \mathbf{x}^{(3)}. \tag{4.4}$$

The unnormalized distribution is consequently a density in second and fourth powers of the variable $\mathbf{x}^{(1)}$, $\mathbf{x}^{(2)}$ while the variables $\mathbf{x}^{(3)}$ appear as arguments of trigonometric functions. This density is subsequently substituted into (3.3) to find the *a posteriori* probability distribution for θ. Although this example is quite simple, it serves to illustrate the basic principles; a fully coupled Hamiltonian matrix would require numerical analysis.

It is difficult to analytically reduce this distribution, but it is possible to obtain information on the asymptotic behavior of the associated estimator via the Rao–Cramer lower bound introduced in the Sec. III. In the present case the matrix is given by (3.6), where

$$\left(\frac{\partial}{\partial\theta_p}\mathbf{G}(s)\right)_k = \sum_{i,j=1}^{L} O_{kij}\left[\mathrm{Re}\left(\frac{\partial}{\partial\theta_p}v_i(s)\right)v_j^*(s)\right]. \tag{4.5}$$

Suppose for the moment that the tensor O_{kij} is a diagonal matrix for all k, then (3.6) and (4.5) show that the diagonal elements of the matrix Z become

$$(Z)_{2L+p\,2L+p} = \frac{1}{\gamma^2}\int_0^s d\tau\sum_{k=1}^{M}\left[\frac{\partial}{\partial\alpha_p}\sum_{i=1}^{L} O_{kii}\{|v_i(\tau)|^2\}\right]^2 = 0, \tag{4.6}$$

because $|v_i(\tau)|^2$, $i = 1,...,L$, is a conserved quantity. Hence no information on the parameter can be derived from the observations if both the Hamiltonian matrix is diagonal and if the matrices O_{kij} are diagonal for every $k = 1,...,M$.

Consider now an example where the elements O_{kij} are diagonal except for the elements O_{kij}, $i = k'-1, k', k'+1$, $j = k'-1, k', k'+1$. Then we find

$$(Z)_{2L+p\,2L+p} = \frac{1}{\gamma^2}\int_0^s d\tau \sum_{k=1}^{M}\left[\frac{\partial}{\partial\alpha_p}\sum_{i}^{L} O_{ki}\{|v_i(\tau)|^2\}\right]^2$$

$$+\frac{1}{\gamma^2}\int_0^s d\tau \sum_{k=1}^{M}\left[\sum_{\substack{i=k'-1\\ j=k'-1\\ i\neq j}}^{\substack{i=k'-1\\ j=k'-1}} O_{kij}\{\mathrm{Re}[v_i(0)^{*} v_j(0)\tau\exp[i\tau(\alpha_i-\alpha_j)]](\delta_{ip}-\delta_{jp})\}\right]^2$$

$$\approx \frac{s^3}{6\gamma^2}\sum_{\substack{i,j=k'-1\\ i\neq j\\ k=1,\ldots,M}}^{i,j=k'+1}[O_{kij}\{(\theta_i\theta_j)^2+(\theta_{L+i}\theta_{L+j})^2\}]^2+[O_{kij}\{(\theta_i\theta_{L+j})^2-(\theta_{L+i}\theta_j)^2\}]^2, \tag{4.7}$$

so that the rate at which the information is gained is proportional to the fourth power of the initial conditions and is cubic in time. The rate with which information is gained on the parameters α does not depend on the value of the parameters, but only on the initial expansion coefficients $\theta_1,\ldots,\theta_{2L}$ and on the off-diagonal elements of the matrices θ_{kij}, $k=1,\ldots,M$. It is easy to see that this is also true if all the O_{kij} are nonzero as long as H is a diagonal matrix. The off-diagonal matrix elements of the lower bound matrix Z in this example are not necessarily small, so that the variance is not proportional to the inverse of the diagonal elements but the exact matrix elements can be easily calculated.

In the more general case where H is a full matrix we determine the matrix Z as follows. Introduce matrices O_k, $k=1,\ldots,M$, such that $(\mathsf{O}_k)_{ij}=O_{kij}$ for all k,i,j. Then from (4.5) we have for all $p=1,\ldots,2L+K$,

$$\frac{\partial}{\partial\theta_p}(\mathbf{G}(s))_k = \frac{\partial}{\partial\theta_p}(\mathbf{v}^T\mathsf{O}_k\mathbf{v}^{*}) . \tag{4.8}$$

Let ξ_j, $j=1,\ldots,L$, be the eigenvectors of H and let η_j, $j=1,\ldots,L$, be the corresponding eigenvalues. Since H is real and symmetric the eigenvalues are real. The solution to (2.1) can be written as

$$\mathbf{v}(s) = \sum_{j=1}^{L} c_j\exp(i\eta_j s)\xi_j , \tag{4.9}$$

where the constants c_j are such that $\Sigma_{j=1}^{L} c_j\xi_j = \mathbf{v}(0)$. Hence

$$(Z)_{pq} = \int_0^s d\tau\sum_{k=1}^{M}\left[\sum_{j=1}^{L}\sum_{j'=1}^{L}\frac{\partial}{\partial\theta_p}\right.$$
$$\times[c_jc_{j'}\exp[i(\eta_j-\eta_{j'})\tau](\xi_j^T\mathsf{O}_k\xi_{j'}^{*})]$$
$$\cdot\sum_{r=1}^{L}\sum_{r'=1}^{L}\frac{\partial}{\partial\theta_q}[c_rc_{r'}\exp[i(\eta_r-\eta_{r'})\tau]$$
$$\left.\times(\xi_r^T\mathsf{O}_k\xi_{r'}^{*})]\right] . \tag{4.10}$$

Using only the dominant terms we see that as time becomes large,

$$(Z)_{pq}\simeq\int_0^s d\tau\sum_{\substack{j,j'=1\\ k=1,\ldots,M}}^{j,j'=1}\left\{\tau^2c_j^2c_{j'}^2\frac{\partial}{\partial\theta_p}(\eta_j-\eta_{j'})\right.$$
$$\left.\cdot\frac{\partial}{\partial\theta_p}(\eta_j-\eta_{j'})(\xi_j\mathsf{O}_k\xi_{j'})^2\right\} , \tag{4.11}$$

so that in the general case the matrix Z is proportional to the fourth power in the initial conditions and the third power in time. Since the behavior of the covariance matrix of the estimates is inversely proportional to the matrix in (4.11), we conclude that for the full Hamiltonian, *the variance of the parameter estimates is inversely proportional to the third power of the time and the fourth power of the initial conditions.*

V. CONCLUSIONS AND SUMMARY

This paper proposes to invert experimental data of quantum systems by first representing the observations as a realization of a stochastic variable whose stochastic characteristics incorporate laboratory uncertainties and then applying filtering theory to estimate the unknown parameters from this realization. The drift term in the observational equations was bilinear in the expansion coefficients to include real measurables. The minimum variance estimator for the parameters was calculated analytically for the case that no noise in the quantal system was present while the associated Rao–Cramer lower bound showed that information on the parameters was gained as a third power in time and a fourth power in the initial conditions.

The examples in Sec. III showed that the *a posteriori* probability distribution requires calculations involving the complete variable space whose dimension is twice the number of expansion coefficients plus the number of unknown parameters. The total number of points necessary to establish a probability distribution numerically obeys a power law in the number of parameters, so approximation methods or efficient computer storage techniques will become necessary in the case of a large system. It is advantageous to restrict the calculations as much as possible to a marginal distribution of the parameters in the Hamiltonian, and in many practical problems the potential does not contain many unknowns.

The random element introduced in the model equations (2.5a) can occur in many different ways. Random fluctuations in macroscopic systems can be combined with quantum mechanical systems[11]; for instance, the potential may contain a random term. In addition, there exists a relationship between ergodic theory and quantal systems that introduces stochasticity.[12]

In the inversion of the observational data the estimation process depends on the variance of the fluctuations γ^2. In many applications this constant may be sufficiently small so that the behavior of the estimator in the asymptotic limit $\gamma\to 0$ becomes of interest. This small noise approximation is rather well developed in the systems literature[1,13,14] and consequently can be fruitfully applied to parameter estimation in quantal systems.

An issue we left aside here is the estimation of the noise level, which so far was assumed to be known. Several algor-

ithms have been proposed to estimate the noise level concurrently with the estimation of the state.[1] Such adaptive techniques have been developed in system theory and can be applied to the parameter estimation problem in Sec. II.

The technique suggested in this paper has certain advantages over the more conventional method of minimum least-squares fitting. In addition to the fact that it avoids the usual problem of finding the absolute minimum via a searching method, it also espouses a special philosophy that encourages one to think in a different way about the model-experiment situation. For instance, in the stochastic estimation setting one does not have to be restricted to Gaussian noise since filtering methods have been developed for Ornstein–Uhlenbeck processes, Poisson processes, and some other stochastic processes. This representation also enables the testing of models[4] using likelihood ratios and can be fruitfully used in the quantum mechanical setting to determine whether or not the current model needs to be amended. Furthermore, designing an optimal experiment is equivalent to the optimization of an observational function in order to maximize the gain in information, and this has been developed especially in the area of communication theory.[4] Finally, it should be added that a considerable number of approximation techniques have resulted from the filtering philosophy and are abundant in the literature.

One central simplification in our arguments relied on the Hamiltonian matrix H and the observational vector being of finite dimension. For the general case where both are infinite dimensional, it is easier to rewrite the problem in terms of the wave function in the Schrödinger equation and assume that the measurements are proportional to the weighted square of the wave function perturbed by a Wiener process. Although filtering methods for such distributed parameter systems have been developed, the details are more involved and will be left to future research.

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Perturbative results from the 1/N expansion for screened Coulomb potentials

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The energy eigenvalues for the Hulthén, Yukawa, and exponential-cosine screened Coulomb potentials are calculated in the $1/N$ expansion. States with up to three nodes in the wave functions are considered. We obtain the perturbative results up to the order of λ^8, where λ is the screening parameter.

I. INTRODUCTION

The $1/N$ expansion,[1-3] where N is the number of spatial dimensions, is a powerful tool in solving the Schrödinger equation for spherically symmetric potentials. Its nonperturbative character (in the sense that is not an expansion in a coupling constant) and the simple algebraic recursive computations involved are definite advantages. Furthermore, approximate analytic expressions for the wave functions can also be obtained along with the energy eigenvalues within the same calculational procedure.

Several investigations[4-9] of some common potentials have been carried out with the $1/N$ expansion technique, and remarkably accurate results are obtained. It has also been pointed out that a shift in the natural expansion parameter $k = N + 2l$, where l is the eigenvalue of the N-dimensional orbital angular momentum, can be exploited to yield simple analytic expressions and improved convergence for the energy eigenvalues.[5,6]

In this paper, we present a detailed study of a class of screened Coulomb potentials[10] within the framework of the $1/N$ expansion. The method used is a variant of the standard $1/N$ expansion,[1] and, when implemented in an algebraic manipulation program, provides an extremely simple way of computing the perturbative approximation to the energy eigenvalues and wave functions. States with up to three nodes in the wave function are considered, although only the energy eigenvalues are presented here.

In Sec. II, we briefly review the $1/N$ expansion for spherically symmetric potentials. Formulation for states with m nodes in the wave function is given in Sec. III. Our modified expansion for the case of screened Coulomb potentials are pointed out in Sec. IV. We then discuss in Sec. V results for the Hulthén, Yukawa, and exponential-cosine screened Coulomb (ECSC) potentials. Finally we present the conclusions in Sec. VI.

The computations presented here were carried out using the algebraic manipulation program REDUCE[11] running on an IBM 3081-KX2 computer.

II. THE 1/N EXPANSION FOR THE NODELESS STATES OF A SPHERICALLY SYMMETRIC POTENTIAL

The radial Schrödinger equation for a spherically symmetric potential in N spatial dimensions is (we use units such that $\hbar = c = m = 1$)

$$\left\{-\frac{1}{2}\left(\frac{d^2}{dr^2}+\frac{N-1}{r}\frac{d}{dr}\right)+\frac{l(l+N-2)}{2r^2}+V_N(r)\right\}\phi(r) = E\phi(r)\,, \tag{2.1}$$

where $V_N(r)$ is the N-dimensional potential. Setting

$$\psi(r) = r^{(N-1)/2}\phi(r)\,, \tag{2.2}$$

we have

$$-\frac{1}{2}\frac{d^2}{dr^2}+k^2\left[\frac{1}{8r^2}\left(1-\frac{1-\Delta}{k}\right)\left(1-\frac{3-\Delta}{k}\right)+\hat{V}(r)\right]\psi(r) = E\psi(r)\,, \tag{2.3}$$

where

$$k \equiv N + 2l - \Delta, \quad \hat{V}(r) \equiv V_N(r)/k^2\,,$$

and Δ is a suitable shift, which will be discussed later. In the large k limit, the energy eigenvalue can be approximated by

$$k^2\tilde{E}^{(-2)} \equiv k^2(1/8r_0^2 + \hat{V}(r_0))\,, \tag{2.4}$$

where r_0 is the minimum of the effective potential

$$1/8r^2 + \hat{V}(r)\,.$$

Defining now

$$\tilde{V}(r) \equiv k^2\left[\frac{1}{8r^2}\left(1-\frac{1-\Delta}{k}\right)\times\left(1-\frac{3-\Delta}{k}\right)+\hat{V}(r)\right]-k^2E^{(-2)}\,,$$

$$\tilde{E} \equiv E - k^2\tilde{E}^{(-2)}, \quad x \equiv r - r_0\,,$$

we write the wave function in the form

$$\psi(r) = e^{U(x)}\,. \tag{2.5}$$

Equation (2.3) then becomes

$$-\tfrac{1}{2}[U''(x) + U'(x)U'(x)] + \tilde{V}(x) - \tilde{E} = 0\,. \tag{2.6}$$

The prime denotes differentiation with respect to x. We then substitute the expansions

$$U'(x) = \sum_{n=-1}^{\infty} u^{(n)}(x)k^{-n}\,, \tag{2.7}$$

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$$\tilde{V}(x)=\sum_{n=-2}^{\infty}\tilde{v}^{(n)}(x)k^{-n}, \tag{2.8}$$

$$\tilde{E}=\sum_{n=-1}^{\infty}\tilde{E}^{(n)}k^{-n} \tag{2.9}$$

in (2.6) and demand that the equation be satisfied order by order in k. The following recursive algebraic equations are obtained:

$$u^{(-1)}(x)u^{(-1)}(x)-2\tilde{v}^{(-2)}(x)=0, \tag{2.10}$$

$$u^{(-1)}(x)u^{(0)}(x)+\tilde{E}^{(-1)}-v^{(-1)}+\tfrac{1}{2}u^{(-1)\prime}(x)=0, \tag{2.11}$$

and

$$u^{(-1)}(x)u^{(n+1)}(x)+\tilde{E}^{(n)}-P^{(n)}(x)=0, \tag{2.12}$$

$$P^{(n)}(x)\equiv\tilde{v}^{(n)}(x)-\frac{1}{2}\left[u^{(n)\prime}(x)+\sum_{j=0}^{n}u^{(j)}(x)u^{(n-j)}(x)\right], \quad n=0,1,2,\ldots. \tag{2.13}$$

Each of these equations can be solved consecutively to obtain

$$u^{(-1)}(x)=-\sqrt{2\tilde{v}^{(-2)}(x)}, \tag{2.14}$$

$$\tilde{E}^{(-1)}=\tilde{v}^{(-1)}(0)-\tfrac{1}{2}u^{(-1)\prime}(0), \tag{2.15}$$

$$u^{(0)}(x)=[\tilde{v}^{(-1)}(x)-\tfrac{1}{2}u^{(-1)\prime}(0)-\tilde{E}^{(-1)}]/u^{(-1)}(x), \tag{2.16}$$

and

$$\tilde{E}^{(n)}=P^{(n)}(0), \tag{2.17}$$

$$u^{(n+1)}(x)=[P^{(n)}(x)-\tilde{E}^{(n)}]/u^{(-1)}(x), \tag{2.18}$$

for $n=0,1,2,\ldots$. With the choice $\Delta=0$, and for $\tilde{v}^{(n)}(x)=0$, $n\geq 1$, the scheme of Mlodinow and Shatz[1] is recovered. Another scheme[5,6] is to choose Δ such that $E^{(-1)}$ vanishes, and hopefully the energy eigenvalue series will then have improved convergence. The physical results are obtained upon setting $N=3$ in the energy and wave-function series.

III. FORMULATION FOR STATES WITH m NODES IN THE WAVE FUNCTIONS

For states with m nodes in the wave function, we write explicitly

$$\psi_m(x)=f_m(x)e^{U_m(x)}, \tag{3.1}$$

where $f_m(x)$ is a polynomial of degree m. Substituting this into the Schrödinger equation gives

$$f_m(x)\{\tilde{V}(x)-\tfrac{1}{2}[U_m''(x)+(U_m'(x))^2]-\tilde{E}_m\}-f_m'(x)U_m'(x)-\tfrac{1}{2}f_m''(x)=0. \tag{3.2}$$

We then make the following $1/k$ expansions:

$$\tilde{V}(x)=\sum_{n=-2}^{\infty}\tilde{v}^{(n)}(x)k^{-n}, \tag{3.3}$$

$$\tilde{E}_m=\sum_{n=-1}^{\infty}\tilde{E}_m^{(n)}k^{-n}, \tag{3.4}$$

$$U_m'(x)=\sum_{n=-1}^{\infty}u_m^{(n)}(x)k^{-n}, \tag{3.5}$$

and

$$f_m(x)=x^m+\sum_{n=1}^{\infty}f_m^{(n)}(x)k^{-n}, \tag{3.6}$$

where

$$f_m^{(n)}(x)=\sum_{j=0}^{m-1}a_{m,j}^{(n)}x^j, \quad n\geq 1. \tag{3.7}$$

Looking at Eq. (3.2) order by order $1/k$, we find

$$u_m^{(-1)}(x)u_m^{(-1)}(x)-2\tilde{v}^{(-2)}(x)=0, \tag{3.8}$$

$$u_m^{(-1)}(x)u_m^{(0)}(x)+E_m^{(-1)}-\tilde{v}^{(-1)}(x)+\tfrac{1}{2}u_m^{(-1)\prime}(x)+mx^{m-1}u_m^{(-1)}(x)=0, \tag{3.9}$$

and for $n=0,1,2,\ldots$,

$$x^m[u_m^{(-1)}(x)u_m^{(n+1)}(x)+E_m^{(n)}-P_m^{(n)}(x)]-\sum_{j=1}^{n+1}f_m^{(j)}(x)[Q_m^{(n-j)}(x)-E_m^{(n-j)}]+\sum_{j=0}^{n+1}f_m^{(j)\prime}(x)u_m^{(n-j)}(x)+\frac{1}{2}f_m^{(n)\prime}(x)=0, \tag{3.10}$$

where

$$P_m^{(n)}(x)=\tilde{v}^{(n)}(x)-\frac{1}{2}\left[u_m^{(n)\prime}(x)+\sum_{j=0}^{n}u_m^{(j)}(x)u_m^{(n-j)}(x)\right], \tag{3.11}$$

$$Q_m^{(n)}(x)=P_m^{(n)}(x)-u_m^{(-1)}(x)u_m^{(n+1)}(x). \tag{3.12}$$

The equations are again solved consecutively. We shall demonstrate the solution for the first few orders. From Eq. (3.8) we have

$$u_m^{(-1)}(x)=-\sqrt{2\tilde{v}^{(-2)}(x)}, \tag{3.13}$$

and since $u_m^{(-1)}(0)=0$, we can differentiate Eq. (3.9) once with respect to x and evaluate at $x=0$ to obtain

$$\tilde{E}_m^{(-1)}=\tilde{v}^{(-1)}(0)-(m+\tfrac{1}{2})u_m^{(-1)\prime}(0). \tag{3.14}$$

We then have

$$u_m^{(0)}(x)=\frac{xD_m^{(-1)}(x)-mu_m^{(-1)}(x)}{xu_m^{(-1)}(x)}, \tag{3.15}$$

where

$$D_m^{(-1)}(x)\equiv\tilde{v}^{(-1)}(x)-\tfrac{1}{2}u_m^{(-1)\prime}(x)-\tilde{E}_m^{(-1)}. \tag{3.16}$$

Notice that although $u_m^{(-1)}(x)$ vanishes at $x=0$, the expression for $u_m^{(0)}(x)$ is actually regular at $x=0$.

To the k^0 order, we have

$$x^m[u_m^{(-1)}(x)u_m^{(1)}(x)+\tilde{E}_m^{(0)}-P_m^{(0)}]-f_m^{(1)}(x)[Q_m^{(-1)}(x)-\tilde{E}_m^{(-1)}]+mx^{m-1}u_m^{(0)}(x)-f_m^{(1)\prime}(x)u_m^{(-1)}(x)-\tfrac{1}{2}m(m-1)x^{m-2}=0. \tag{3.17}$$

Evaluating at $x=0$ gives

$$a_{m,0}^{(1)}=\frac{\delta_{m1}u_m^{(0)}(0)+\delta_{m2}}{mu_m^{(-1)\prime}(0)}, \tag{3.18}$$

where δ_{mn} is the Kronecker delta. Differentiating the equation with respect to x l times and evaluating at $x=0$ allow

$a_{m,l}^{(1)}$ to be determined. Once $f_m^{(1)}(x)$ is constructed, the only remaining unknown function in the equation is $u_m{}^{(1)}(x)$, which can then be solved. The same procedure of solution can then be applied to the next order in $1/k$.

IV. THE SCREENED COULOMB POTENTIALS

For the class of screened Coulomb potentials under consideration (the Hulthén, Yukawa, and exponential-cosine screened potentials), we have the power series expansion

$$V(r) = -\frac{Z}{r}\sum_{j=0}^{\infty} V_j(\lambda r)^j, \tag{4.1}$$

where λ is the screening parameter. Scaling the variables Z and λ,

$$Z = k^2\tilde{Z}/4, \quad \lambda = \tilde{\lambda}/k^2, \tag{4.2}$$

we then have the modified potential in N dimensions,

$$V_N(r) = \sum_{n=-2}^{\infty} v^{(n)}(r)k^{-n}, \tag{4.3}$$

where

$$v^{(-2)}(r) = -\tfrac{1}{4}\tilde{Z}/r, \tag{4.4}$$

$$v^{(2j)}(r) = \eta^{(2j)}\tilde{Z}\tilde{\lambda}^{j+1}r^j, \quad j = 0,1,2,\ldots, \tag{4.5}$$

with $\eta^{(2j)}$ being constants. The effective potential in the large k limit in this case is $1/8r^2 - \tilde{Z}/4r$, and the minimum occurs at $r_0 = \tilde{Z}^{-1}$. The general potential (2.8) can then be constructed and the energy eigenvalues and wave functions obtained through Eqs. (2.14)–(2.17) on Eqs. (3.8)–(3.10).

It is obvious from the above discussions that in the present scheme the screened Coulomb potentials are all taken to be approximated by the Coulomb potential in the large k limit. The screening effects are then computed as higher-order corrections in the $1/k$ expansion. The advantages are the explicit and simple expressions can be obtained for the minimum position r_0 and the function $u^{(-1)}(x)$, which is the starting point of the recursive calculational procedure. The price that has to be paid is that only perturbative results are obtained.

We perform the general computations using the algebraic manipulation program REDUCE[11] and results for the individual cases are obtained by assigning appropriate numerical values to the V_j's in (4.1). As a check of our program and to verify that the standard $1/N$ expansion is intrinsically nonperturbative, we calculate the energy eigenvalues and the associated wave functions for the limiting Coulomb case using the same REDUCE program and setting the screening parameter λ to zero. We find, for $N = 3$,

$$E_m = \sum_{j=-2}^{\infty} \tilde{E}_m{}^{(j)}k^{-j}, \tag{4.6}$$

where m is the number of nodes in the wave function, and

$$\tilde{E}_m{}^{(j)} = -\tfrac{1}{8}\tilde{Z}^2(-1)^j(j+3)(\Delta - 1 + 2m)^{j+2}, \tag{4.7}$$

for $0 \leqslant j \leqslant 25$. We believe that (4.7) will continue to hold for $j > 25$. Writing $\zeta_m = -(\Delta - 1 + 2m)/k$, we then have

$$E_m = -\frac{1}{8}\tilde{Z}^2k^2\sum_{j=0}^{\infty}(j+1)(\zeta_m)^j, \tag{4.8}$$

which, for $|\zeta| < 1$, is

$$E_m = -\tfrac{1}{8}\tilde{Z}^2k^2[1/(1-\zeta)^2]$$

$$\underset{N\to 3}{\to} -Z^2/2(m+l+1)^2 = -Z^2/2n^2, \tag{4.9}$$

which are the exact expressions for the energy eigenvalues for the Coulomb potential, with $n = (m + l + 1)$ being the principal quantum number. This result is *independent* of the choice of the shift parameter Δ. Of course, with $\Delta_m = 1 - 2m$, the energy eigenvalues are then given simply by

$$E_m = \tilde{E}^{(-2)}k^2 = -\tfrac{1}{8}\tilde{Z}^2(N + 2l + 2m - 1)^2$$

$$\underset{N\to 3}{\to} -\tfrac{1}{2}Z^2/(m+l+1)^2 = -Z^2/2n^2, \tag{4.10}$$

as expected.

Apart from the normalization factor, exact r dependence of the reduced radial wave functions, $rR_{nl}(r)$, is also reproduced in the calculation. Explicitly, we find for $Z = 1$, $\Delta_m = 1 - 2m$, and $N = 3$,

$$U_{m=0}(x) = -x/n + n\ln[(x - n^2)/n^2], \tag{4.11}$$

$$U_{m=1}(x) = (x+n) \times\{-x/n + (n-1)\ln[(x+n^2)/n^2]\}, \tag{4.12}$$

$$U_{m=2}(x) = \tfrac{1}{2}(2x^2 + 6nx - n^3 + 6n^2) \times\{-x/n + (n-2)\ln[(x-n^2)/n^2]\}, \tag{4.13}$$

$$U_{m=3}(x) = \tfrac{1}{2}[2x^3 + 12nx^2 - 3n^2(n-10)x - 7n^4 + 30n^3] \times\{-x/n + (n-3)\ln[(x-n^2)/n^2]\}, \tag{4.14}$$

which, when exponentiated, and recalling that

$$r_0 = \tfrac{1}{4}(3 + 2l - \Delta_m)^2 = n^2, \tag{4.15}$$

give the correct r dependence of the reduced radial wave functions for the $1s$ through $4f$ states.

V. RESULTS FOR THE HULTHÉN, YUKAWA, AND ECSC POTENTIALS

The constants $\eta^{(2j)}$ in (4.5) for the Hulthén, Yukawa, and exponential-cosine screened Coulomb (ECSC) potentials are listed in Table I. Analytic expressions for the $N = 3$

TABLE I. The constants $\eta^{(2j)}$ for the Hulthén, Yukawa, and ECSC potentials.

	Hulthén	Yukawa	ECSC
$\eta^{(0)}$	$\frac{1}{2}$	1	1
$\eta^{(2)}$	$-\frac{1}{48}$	$-\frac{1}{8}$	0
$\eta^{(4)}$	0	$+\frac{1}{24}$	$-\frac{1}{12}$
$\eta^{(6)}$	$+\frac{1}{2880}$	$-\frac{1}{96}$	$+\frac{1}{24}$
$\eta^{(8)}$	0	$+\frac{1}{480}$	$+\frac{1}{120}$
$\eta^{(10)}$	$-\frac{1}{120\,960}$	$-\frac{1}{2880}$	0
$\eta^{(12)}$	0	$+\frac{1}{20\,160}$	$+\frac{1}{2520}$
$\eta^{(14)}$	$+\frac{1}{4838\,400}$	$-\frac{1}{161\,280}$	$-\frac{1}{10\,080}$

TABLE II. Analytic expressions for the energy eigenvalues as power series in the screening parameter λ.

(a) Hulthén potential

$$E_{ns} = -(1/2n^2) + \tfrac{1}{2}\lambda - \tfrac{1}{8}n^2\lambda^2, \quad n = 1,2,3,4$$

$$E_{2p} = -\tfrac{1}{8} + \tfrac{1}{2}\lambda - \tfrac{5}{12}\lambda^2 - \tfrac{1}{8}\lambda^4 - \tfrac{19}{72}\lambda^6 - \tfrac{37}{432}\lambda^8$$

$$E_{3p} = -\tfrac{1}{18} + \tfrac{1}{2}\lambda - \tfrac{25}{24}\lambda^2 - \tfrac{3}{4}\lambda^4 - \tfrac{363}{64}\lambda^6 - \tfrac{178\,659}{2\,560}\lambda^8$$

$$E_{3d} = -\tfrac{1}{18} + \tfrac{1}{2}\lambda - \tfrac{7}{8}\lambda^2 - \tfrac{63}{40}\lambda^4 - \tfrac{5589}{320}\lambda^6 - \tfrac{3\,734\,667}{12\,800}\lambda^8$$

$$E_{4p} = -\tfrac{1}{32} + \tfrac{1}{2}\lambda - \tfrac{23}{12}\lambda^2 - \tfrac{5}{2}\lambda^4 - \tfrac{460}{9}\lambda^6 - \tfrac{81\,392}{45}\lambda^8$$

$$E_{4d} = -\tfrac{1}{32} + \tfrac{1}{2}\lambda - \tfrac{7}{4}\lambda^2 - \tfrac{63}{10}\lambda^4 - \tfrac{864}{5}\lambda^6 - \tfrac{182\,104}{25}\lambda^8$$

$$E_{4f} = -\tfrac{1}{32} + \tfrac{1}{2}\lambda - \tfrac{3}{2}\lambda^2 - 9\lambda^4 - \tfrac{2208}{7}\lambda^6 - \tfrac{585\,976}{35}\lambda^8$$

(b) Yukawa potential

$$E_{1s} = -\tfrac{1}{2} + \lambda - \tfrac{3}{4}\lambda^2 + \tfrac{1}{2}\lambda^3 - \tfrac{11}{16}\lambda^4 + \tfrac{21}{16}\lambda^5 - \tfrac{145}{48}\lambda^6 + \tfrac{757}{96}\lambda^7 - \tfrac{69\,433}{3072}\lambda^8$$

$$E_{2s} = -\tfrac{1}{8} + \lambda - 3\lambda^2 + 7\lambda^3 - \tfrac{121}{4}\lambda^4 + 186\lambda^5 - \tfrac{8239}{6}\lambda^6 + \tfrac{34\,414}{3}\lambda^7 - \tfrac{1256\,135}{12}\lambda^8$$

$$E_{2p} = -\tfrac{1}{8} + \lambda - \tfrac{5}{2}\lambda^2 + 5\lambda^3 - \tfrac{95}{4}\lambda^4 + 144\lambda^5 - \tfrac{6431}{6}\lambda^6 + \tfrac{26\,570}{3}\lambda^7 - \tfrac{959\,575}{12}\lambda^8$$

$$E_{3s} = -\tfrac{1}{18} + \lambda - \tfrac{27}{4}\lambda^2 + \tfrac{69}{2}\lambda^3 - \tfrac{5049}{16}\lambda^4 + \tfrac{65\,043}{16}\lambda^5 - \tfrac{994\,437}{16}\lambda^6 + \tfrac{34\,182\,081}{32}\lambda^7 - \tfrac{20\,438\,702\,541}{1024}\lambda^8$$

$$E_{3p} = -\tfrac{1}{18} + \lambda - \tfrac{25}{4}\lambda^2 + 30\lambda^3 - \tfrac{2295}{8}\lambda^4 + \tfrac{29\,403}{8}\lambda^5 - \tfrac{449\,307}{8}\lambda^6 + \tfrac{7\,672\,725}{8}\lambda^7 - \tfrac{9\,115\,776\,855}{512}\lambda^8$$

$$E_{3d} = -\tfrac{1}{18} + \lambda - \tfrac{21}{4}\lambda^2 + 21\lambda^3 - \tfrac{1701}{8}\lambda^4 + \tfrac{20\,979}{8}\lambda^5 - \tfrac{322\,623}{8}\lambda^6 + 677\,970\lambda^7 - \tfrac{6\,379\,437\,447}{512}\lambda^8$$

$$E_{4s} = -\tfrac{1}{32} + \lambda - 12\lambda^2 + 108\lambda^3 - 1716\lambda^4 + 38\,160\lambda^5 - 999\,584\lambda^6$$

$$E_{4p} = -\tfrac{1}{32} + \lambda - \tfrac{23}{2}\lambda^2 + 100\lambda^3 - 1630\lambda^4 + 36\,144\lambda^5 - \tfrac{2836\,352}{3}\lambda^6 + \tfrac{82\,697\,920}{3}\lambda^7 - \tfrac{2609\,134\,640}{3}\lambda^8$$

$$E_{4d} = -\tfrac{1}{32} + \lambda - \tfrac{21}{2}\lambda^2 + 84\lambda^3 - 1428\lambda^4 + 31\,248\lambda^5 - 817\,936\lambda^6 + 23\,637\,440\lambda^7 - 739\,863\,280\lambda^8$$

$$E_{4f} = -\tfrac{1}{32} + \lambda - 9\lambda^2 + 60\lambda^3 - 1050\lambda^4 + 21\,744\lambda^5 - 567\,664\lambda^6 + 16\,028\,480\lambda^7 - 495\,437\,680\lambda^8$$

(c) ECSC potential

$$E_{1s} = -\tfrac{1}{2} + \lambda - \lambda^3 + \tfrac{5}{4}\lambda^4 - \tfrac{3}{4}\lambda^5 - \tfrac{43}{12}\lambda^6 + \tfrac{49}{3}\lambda^7 - \tfrac{6505}{192}\lambda^8$$

$$E_{2s} = -\tfrac{1}{8} + \lambda - 14\lambda^3 + 55\lambda^4 - 96\lambda^5 - \tfrac{4928}{3}\lambda^6 + \tfrac{65\,352}{3}\lambda^7 - \tfrac{385\,280}{3}\lambda^8$$

$$E_{2p} = -\tfrac{1}{8} + \lambda - 10\lambda^3 + 35\lambda^4 - 56\lambda^5 - \tfrac{3520}{3}\lambda^6 + \tfrac{42\,160}{3}\lambda^7 - \tfrac{227\,660}{3}\lambda^8$$

$$E_{3s} = -\tfrac{1}{18} + \lambda - 69\lambda^3 + \tfrac{2295}{4}\lambda^4 - \tfrac{8181}{4}\lambda^5 - \tfrac{297\,999}{4}\lambda^6 + 1989\,441\lambda^7 - \tfrac{1\,479\,931\,965}{64}\lambda^8$$

$$E_{3p} = -\tfrac{1}{18} + \lambda - 60\lambda^3 + \tfrac{945}{2}\lambda^4 - \tfrac{3213}{2}\lambda^5 - \tfrac{129\,195}{2}\lambda^6 + \tfrac{3\,269\,565}{2}\lambda^7 - \tfrac{580\,878\,135}{32}\lambda^8$$

$$E_{3d} = -\tfrac{1}{18} + \lambda - 42\lambda^3 + \tfrac{567}{2}\lambda^4 - \tfrac{1701}{2}\lambda^5 - \tfrac{84\,483}{2}\lambda^6 + \tfrac{1\,891\,755}{2}\lambda^7 - \tfrac{302\,376\,807}{32}\lambda^8$$

TABLE II. (*Continued.*)

$$E_{4s} = -\tfrac{1}{32} + \lambda - 216\lambda^3 + 3120\lambda^4 - 19\,008\lambda^5 - 1199\,104\lambda^6$$

$$E_{4p} = -\tfrac{1}{32} + \lambda - 200\lambda^3 + 2800\lambda^4 - 16\,576\lambda^5 - \tfrac{3322\,880}{3}\lambda^6 + \tfrac{144\,909\,824}{3}\lambda^7 - \tfrac{2734\,908\,160}{3}\lambda^8$$

$$E_{4d} = -\tfrac{1}{32} + \lambda - 168\lambda^3 + 2184\lambda^4 - 12\,096\lambda^5 - 910\,336\lambda^6 + 37\,023\,232\lambda^7 - 656\,936\,704\lambda^8$$

$$E_{4f} = -\tfrac{1}{32} + \lambda - 120\lambda^3 + 1320\lambda^4 - 6336\lambda^5 - 578\,560\lambda^6 + 20\,720\,128\lambda^7 - 328\,472\,320\lambda^8$$

energy eigenvalues as a function of the screening parameter λ are given in Table II. In our calculations we have chosen the units with $m = \hbar = c = Z = 1$, and a shift parameter $\Delta_m = 1 - 2m$ for the m-node state is adopted. As discussed in Sec. IV, this choice allows the Coulomb limit result to be reproduced at the $\tilde{E}^{(-2)}$ level. In most cases, the calculations are carried out in high enough orders (in $1/k$) to ensure that convergence to order λ^8 has been achieved. For the three-node $4s$ state however, only results correct to λ^6 are obtained due to computer memory limitations.

It has been pointed out in Ref. 12 that the energy levels of some screened Coulomb potentials have an asymptotic series in λ, indicating that any finite-order perturbation calculation cannot be expected to yield results of arbitrary accuracy in such cases. The Padé approximant method[13,14] has been particularly successful in circumventing this difficulty.[15–18] In our present study, we shall only perform simple iterated Shanks transformations[14] on our results as a check on their convergence.

For the Hulthén potential, exact expressions[19] for the energy eigenvalues of the $l = 0$ states are reproduced, whereas for the $l \neq 0$ states, we agree with Ref. 18 up to λ^6. Numerical values for these eigenvalues are given in Tables III–V, along with results from the other calculations. The values $E12$ and $E6$ are, respectively, eigenvalues correct to the twelfth and sixth orders in λ. The $E8$ are values computed from the energy series given in Table II and are correct to the eighth order in λ. The $E12$, $E6$, and the Padé approximant values are all taken from Ref. 18. Good agreement over a range of values of λ with the Padé approximant results is particularly encouraging. Convergence does not pose a problem in this case except when the screening parameter λ is close to the critical values.

TABLE III. Energy eigenvalues for the $2p$ states of the Hulthén potential in atomic units.

			Present calculation	
λ	$E12$	$E_{\text{Padé}}$	$E8$	E_{Shanks}
0.05	−0.101 043	−0.101 043	−0.101 043	−0.101 043
0.10	−0.079 179	−0.079 179	−0.079 179	−0.079 179
0.20	−0.041 886	−0.041 886	−0.041 886	−0.041 886
0.30	−0.013 784	−0.013 790	−0.013 759	−0.013 785
0.35	−0.003 720	−0.003 779	−0.003 588	−0.003 739

TABLE IV. Energy eigenvalues of the Hulthén potential for the $3p$ and $3d$ states in atomic units.

λ		Present calculation			
		$E6$	$E_{\text{Padé}}$	$E8$	E_{Shanks}
0.025	$3p$	−0.043 707	−0.043 707	−0.043 707	−0.043 707
	$3d$	−0.043 603	−0.043 603	−0.043 603	−0.043 603
0.050	$3p$	−0.033 165	−0.033 165	−0.033 165	−0.033 165
	$3d$	−0.032 753	−0.032 753	−0.032 753	−0.032 753
0.100	$3p$	−0.016 053	−0.016 054	−0.016 054	−0.016 054
	$3d$	−0.041 481	−0.014 484	−0.014 483	−0.014 484
0.150	$3p$	−0.004 437	−0.004 466	−0.004 455	−0.004 464
	$3d$	−0.001 239	−0.001 391	−0.001 314	−0.001 375

TABLE V. Energy eigenvalues of the Hulthén potential for the $4p$, $4d$, and $4f$ states in atomic units.

λ		Present calculation			
		$E6$	$E_{\text{Padé}}$	$E8$	E_{Shanks}
0.025	$4p$	−0.019 949	−0.019 949	−0.019 949	−0.019 949
	$4d$	−0.019 846	−0.019 846	−0.019 846	−0.019 846
	$4f$	−0.019 691	−0.019 691	−0.019 691	−0.019 691
0.050	$4p$	−0.011 058	−0.011 058	−0.011 058	−0.011 058
	$4d$	−0.010 667	−0.010 667	−0.010 667	−0.010 667
	$4f$	−0.010 061	−0.010 062	−0.010 062	−0.010 062
0.075	$4p$	−0.004 619	−0.004 622	−0.004 621	−0.004 622
	$4d$	−0.003 824	−0.003 834	−0.003 831	−0.003 834
	$4f$	−0.002 528	−0.002 556	−0.002 545	−0.002 554
0.100	$4p$	−0.000 718	−0.000 754	−0.000 736	−0.000 751

TABLE VI. Energy eigenvalues of the Yukawa potential for the $1s$ state in atomic units.

λ	Padé approximant		Present calculation	
	$E[6,6]$	$E[6,7]$	$E8$	E_{shanks}
0.10	−0.407 06	−0.407 06	−0.407 06	−0.407 06
0.20	−0.326 81	−0.326 81	−0.326 83	−0.326 81
0.25	−0.290 92	−0.290 92	−0.291 07	−0.290 92
0.50	−0.148 12	−0.148 12	−0.200 84	−0.148 12
0.80	−0.044 71	−0.044 70	−2.705 69	−0.044 75
0.90	−0.024 33	−0.024 31	−7.082 05	−0.024 39
1.00	−0.010 32	−0.010 27	−16.862 31	−0.010 42
1.05	−0.005 60	−0.005 53	−25.204 52	−0.005 73
1.10	−0.002 35	−0.002 25	−36.969 07	−0.002 51
1.15	−0.000 54	−0.000 41	−53.295 67	−0.000 73

TABLE VII. Energy eigenvalues of the Yukawa potential for the $2s$ and $2p$ states in atomic units.

λ		Padé approximant		Present calculation	
		$E[6,6]$	$E[6,7]$	$E8$	E_{Shanks}
0.05	$2s$	−0.081 77	−0.081 77	−0.081 77	−0.081 77
	$2p$	−0.080 74	−0.080 74	−0.080 74	−0.080 74
0.10	$2s$	−0.049 93	−0.049 93	−0.050 44	−0.049 91
	$2p$	−0.046 53	−0.046 53	−0.046 92	−0.046 52
0.20	$2s$	−0.012 11	−0.012 11	−0.186 91	−0.011 55
	$2p$	−0.004 18	−0.004 04	−0.136 86	−0.003 41
0.25	$2s$	−0.003 41	−0.003 39	−1.122 00	−0.002 11
0.30	$2s$	−0.000 17	−0.000 05	−5.059 22	

TABLE VIII. Energy eigenvalues of the Yukawa potential for the 3s, 3p,and 3d states in atomic units.

λ		Padé approximant $E[6,6]$	Padé approximant $E[6,7]$	Present calculation $E8$	Present calculation E_{Shanks}
0.025	3s	−0.034 33	−0.034 33	−0.034 33	−0.034 33
	3p	−0.034 08	−0.034 08	−0.034 08	−0.034 08
	3d	−0.033 57	−0.033 57	−0.033 57	−0.033 57
0.050	3s	−0.019 35	−0.019 35	−0.019 74	−0.019 36
	3p	−0.018 56	−0.018 56	−0.018 90	−0.018 56
	3d	−0.016 92	−0.016 92	−0.017 15	−0.016 92
0.080	3s	−0.007 78	−0.007 78	−0.028 07	−0.007 85
	3p	−0.006 35	−0.006 33	−0.024 38	−0.006 31
	3d	−0.003 25	−0.003 24	−0.015 78	−0.003 25
0.10	3s	−0.003 21	−0.003 21	−0.134 39	−0.003 46
	3p	−0.001 53	−0.001 58	−0.118 29	−0.001 48
012	3s	−0.000 74	−0.000 73	−0.598 48	−0.001 38

The $1/N$ expansion calculations for the Yukawa potential have been carried out before, although attention was confined to the 1s and 2s states.[8,9] Our results as given in Table I indicate that the energy eigenvalues take the form of divergent, or at best asymptotic, power series in λ. Numerical values for E_{1s} in Table VI show that incorrect results are obtained from the perturbative series for $\lambda > 0.25$. Convergence, however, is much improved by the Shanks transformations, although the accuracy achieved still does not match those of the more sophisticated Padé approximants.[15] Results for the other excited states are given in Tables VII–IX, which also include Padé approximant values taken from Ref. 15.

We encounter the worse case of nonconvergence in the energy series for the ECSC potential. Our perturbative results agree with those of Ref. 17 to order λ^5. Although the eigenvalues are not grossly in error over a range of λ values, the convergence of the energy series for each state is not much, if at all, improved by the Shanks transformations. For comparison purposes, we present the numerical values of the energy eigenvalues of the various states in Tables X–XIII, along with results from the other calculations.[16,17] The values E_{exact} are taken from Ref. 16 and correspond to the $E[10,10]$ values computed within the hypervirial Padé scheme. The $E5$ (perturbative result correct to the fifth order in λ) and $E_{\text{Padé}}$ ($E[3,2]$ Padé approximant to $E5$) values are from Ref. 17.

VI. CONCLUSIONS

Using a modified $1/N$ expansion technique, we have exploited the analytic capabilities of algebraic manipulation programs (such as REDUCE used here) to recursively calculate energy eigenvalues and wave functions of the Schrödinger equation for a class of screened Coulomb potentials. The method developed here can be applied to any potential that has the form (4.1). Perturbative results for the Hulthén, Yukawa, and ECSC potentials are obtained. In the cases of the Hulthén and Yukawa potentials, convergence of the energy series can be accelerated using simple iterated Shanks transformations, whereas the more sophisticated Padé approximant method is required to obtain energy levels of high accuracy for the ECSC potential.

TABLE IX. Energy eigenvalues of the Yukawa potential for the 4s, 4p, 4d, and 4f states in atomic units.

λ		Padé approximant $E[6,6]$	Padé approximant $E[6,7]$	Present calculation $E8$	Present calculation E_{Shanks}
0.025	4s	−0.012 50	−0.012 50	−0.012 60[a]	−0.012 50[a]
	4p	−0.012 29	−0.012 29	−0.012 35	−0.012 29
	4d	−0.011 87	−0.011 87	−0.011 92	−0.011 87
	4f				
0.050	4s	−0.003 09	−0.003 09	−0.012 17[a]	−0.003 14[a]
	4p	−0.002 60	−0.002 60	−0.023 60	−0.002 60
	4d	−0.001 57	−0.001 58	−0.019 37	−0.001 51
0.06	4s	−0.001 24	−0.001 24	−0.030 32[a]	−0.001 37[a]
	4p	−0.000 71	−0.000 75	−0.097 09	−0.000 71
0.08	4s	−0.000 05	−0.000 01	−0.180 03[a]	−0.000 58[a]

[a] To order λ^6 only.

TABLE X. Energy eigenvalues of the ECSC potential for the $1s$ state in atomic units.

λ	Padé approximant $E5$	Padé approximant $E[2,3]$	E_{exact}	Present calculation $E8$	Present calculation E_{Shanks}
0.06	− 0.440 200	− 0.440 201	− 0.440 201	− 0.440 201	− 0.440 201
0.08	− 0.420 463	− 0.420 464	− 0.420 464	− 0.420 464	− 0.420 464
0.10	− 0.400 883	− 0.400 884	− 0.400 885	− 0.400 885	− 0.400 886
0.20	− 0.306 240	− 0.306 300	− 0.306 335	− 0.306 347	− 0.307 601
0.30	− 0.218 698	− 0.219 152	− 0.219 416	− 0.219 961	− 0.217 688
0.40	− 0.139 680	− 0.141 389	− 0.142 439	− 0.149 801	− 0.137 282
0.50	− 0.070 313	− 0.074 675	− 0.077 680	− 0.131 042	− 0.063 520

TABLE XI. Energy eigenvalues of the ECSC potential for the $2s$, $2p$ states in atomic units.

λ		E_{exact}	$E_{\text{Padé}}$	$E5$	Present calculation $E8$	Present calculation E_{Shanks}
0.02	$2s$	− 0.105 104	− 0.105 104	− 0.105 104	− 0.105 104	− 0.105 104
	$2p$	− 0.105 075	− 0.105 075	− 0.105 075	− 0.105 075	− 0.105 075
0.04	$2s$	− 0.085 769	− 0.085 769	− 0.085 765	− 0.085 769	− 0.085 774
	$2p$	− 0.085 591	− 0.085 558	− 0.085 556	− 0.085 559	− 0.085 566
0.06	$2s$	− 0.067 421	− 0.067 425	− 0.067 386	− 0.067 423	− 0.066 695
	$2p$	− 0.066 778	− 0.066 771	− 0.066 750	− 0.066 778	− 0.066 717
0.08	$2s$	− 0.050 387	− 0.050 408	− 0.050 230	− 0.050 418	− 0.050 058
	$2p$	− 0.048 997	− 0.048 967	− 0.048 870	− 0.049 010	− 0.048 845
010	$2s$	− 0.034 941	− 0.035 027	− 0.034 460	− 0.035 203	− 0.034 227
	$2p$	− 0.032 469	− 0.032 372	− 0.032 060	− 0.032 587	− 0.032 055

TABLE XII. Energy eigenvalues of the ECSC potential for the $3s$, $3p$, and $3d$ states in atomic units.

λ		E_{exact}	$E_{\text{Padé}}$	$E5$	Present calculation $E8$	Present calculation E_{Shanks}
0.02	$3s$	− 0.036 025	− 0.036 026	− 0.036 022	− 0.036 025	− 0.036 029
	$3p$	− 0.035 968	− 0.035 968	− 0.035 965	− 0.035 968	− 0.035 972
	$3d$	− 0.035 851	− 0.035 850	− 0.035 849	− 0.035 851	− 0.035 952
0.04	$3s$	− 0.018 823	− 0.018 863	− 0.018 712	− 0.018 843	− 0.018 632
	$3p$	− 0.018 453	− 0.018 469	− 0.018 350	− 0.018 466	− 0.018 319
	$3d$	− 0.017 682	− 0.017 669	− 0.017 605	− 0.017 685	− 0.017 614
0.05	$3s$	− 0.011 576	− 0.011 724	− 0.011 234	− 0.011 747	− 0.011 127
	$3p$	− 0.010 929	− 0.010 990	− 0.010 604	− 0.011 046	− 0.010 580
	$3d$	− 0.009 555	− 0.009 511	− 0.009 299	− 0.009 590	− 0.009 349
0.06	$3s$	− 0.005 461	− 0.005 950	− 0.004 614	− 0.006 405	− 0.004 428
	$3p$	− 0.004 471	− 0.004 679	− 0.003 641	− 0.005 128	− 0.003 617
	$3d$	− 0.002 308	− 0.002 180	− 0.001 615	− 0.002 525	− 0.001 743

TABLE XIII. Energy eigenvalues of the ECSC potential for the $4s$, $4p$, $4d$, and $4f$ states in atomic units.

λ		E_{exact}	$E_{\text{Padé}}$	Present calculation $E5$	$E8$	E_{Shanks}
0.01	$4s$	−0.021 438	−0.021 438	−0.021 437	−0.021 438[a]	−0.021 437[a]
	$4p$	−0.021 424	−0.021 425	−0.021 424	−0.021 424	−0.021 425
	$4d$	−0.021 398	−0.021 398	−0.021 397	−0.021 398	−0.021 399
	$4f$	−0.021 358	−0.021 358	−0.021 357	−0.021 358	−0.021 359
0.02	$4s$	−0.012 572	−0.012 582	−0.012 540	−0.012 616[a]	−0.012 565[a]
	$4p$	−0.012 486	−0.012 493	−0.012 455	−0.012 487	−0.012 427
	$4d$	−0.012 310	−0.012 311	−0.012 283	−0.012 311	−0.012 275
	$4f$	−0.012 038	−0.012 035	−0.012 019	−0.012 038	−0.012 022
0.03	$4s$	−0.005 270	−0.005 396	−0.005 017	−0.005 891[a]	−0.005 199[a]
	$4p$	−0.005 033	−0.005 117	−0.004 785	−0.005 134	−0.004 760
	$4d$	−0.004 539	−0.004 559	−0.004 311	−0.004 596	−0.004 333
	$4f$	−0.003 748	−0.003 720	−0.003 574	−0.003 759	−0.003 623

[a]To order λ^6 only.

It should perhaps be pointed out that although the unmodified $1/N$ expansion[1] can generate results that are not perturbative (in λ), the energy series (in $1/k$) is also, although asymptotic, often divergent. Resummation techniques are still necessary to stabilize the sequence of partial sums. Furthermore, calculations in such a case are extremely complicated algebraically, and, even with algebraic manipulation programs, only a limited number of terms in the $1/k$ series can be computed.

After this paper was submitted for publication, it was brought to my attention that similar treatments of the Hulthén potential and the generalized exponential cosine-screened Coulomb potential have recently appeared in the literature.[20,21] I wish to thank the referee for informing me of these references.

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On the complete integrability of the supersymmetric nonlinear Schrödinger equation

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The Painlevé criterion has been applied to the supersymmetric nonlinear Schrödinger equation. This particular system of fermionic and bosonic fields shows up a rich spectrum of resonances and it can be explicitly proved that the expansion coefficients at the resonance positions can remain arbitrary. At this point is is worth noting that even when the extra nonlinear field (which is fermionic in this case) is considered to be bosonic, the resulting system turns out to satisfy the Painlevé test so that this second system may be thought of as a new completely integrable system whose Lax pair is still to be found.

I. INTRODUCTION

In recent times the class of nonlinear integrable equations has been extended in various directions. One of the most important classes is obtained by the incorporation of fermionic fields in accordance with the principle of two-dimensional supersymmetry.[1] The corresponding super-AKNS problem has been worked out very recently. The Bäcklund transformation and Hamiltonian structure of such equations have been obtained by Roy Chowdhury and Roy.[2] Here our motivation is to apply the Painlevé property of such evolution equations containing anticommuting variables, which to the extent of the present authors' knowledge has not yet been done. Incidentally, a new result sprang up from our analysis, that is, if we consider the extra nonlinear variable (ψ) as a bosonic field, rather than a fermionic one, even then the set of equation is completely integrable in the Painlevé sense so that we have actually obtained a new class of coupled nonlinear Schrödinger equations (NLSE's) which is integrable but whose Lax pair is still not known.

II. FORMULATION

The supersymmetric NLSE's read[3]

$$\begin{aligned} iq_t &= -q_{xx} + 2Kq^*q^2 + K\psi^+\psi q - iK^{1/2}\psi\psi_x , \\ i\psi_t &= -2\psi_{xx} + kq^+q\psi - ik^{1/2}(2q\psi_x^+ + \psi^+ q_x) , \end{aligned} \tag{1}$$

where $q(x,t)$ is the original NLSE field variable and $\psi(x,t)$, $\psi^+(x,t)$ are the fermionic counterparts introduced through supersymmetry. In the following we will be working with the real and imaginary parts of (1) so we set

$$q = u_0 + iv_0 , \quad \psi = u_1 + iv_1 , \tag{2}$$

whence we have the four nonlinear partial differential equations

$$\begin{aligned} -v_{0t} &= -u_{0xx} + k\,[2u_0(u_0^2+v_0^2) + v_0(u_1^2+v_1^2)] \\ &\quad + k^{1/2}(v_1u_{1x} + u_1v_{1x}) , \\ -v_{1t} &= -2u_{1xx} + ku_1(u_0^2+v_0^2) \\ &\quad + k^{1/2}[2(v_0u_{1x} - u_0v_{1x}) + (u_1v_{0x} - v_1u_{0x})] , \\ u_{1t} &= -2v_{1xx} + kv_1(u_0^2+v_0^2) \\ &\quad - k^{1/2}[2(u_0u_{1x} + v_0v_{1x}) + (u_1u_{0x} + v_1v_{0x})] . \end{aligned} \tag{3}$$

To proceed with the Painlevé analysis we set[4]

$$\begin{aligned} u_0 &= \sum_{j=0}^{\infty} a_j\phi^{j+\alpha} , \quad v_0 = \sum_{j=0}^{\infty} b_j\phi^{j+\beta} , \\ u_1 &= \sum_{j=0}^{\infty} c_j\phi^{j+\gamma} , \quad v_1 = \sum_{j=0}^{\infty} d_j\phi^{j+\delta} . \end{aligned} \tag{4}$$

At this point we should note that this type of general ansatz was first used by Weiss *et al.*[5] But then a simplification of this ansatz, which at present is widely used, was formulated by Kruskal.[6] He suggested that one can specialize $\phi(x,t)$ as $\phi = x - f(t)$ and consider the expansion coefficients to be functions of "time" only. We are actually following Kruskal's prescription and analyzing the Painlevé conjecture of "pole's being the only movable singularity in the complex t-plane." The most important and successful applications of this simplified ansatz is in the case of the Zakharov equation by Goldstein and Infeld,[7] in the case of the modified Boussinesq equation by Clarkson,[8] in the case of the longwave–shortwave interaction equation by Roy Chowdhury and Chanda,[9] and lastly in the case of the Yang–Mills equation by Jimbo *et al.*[10]

But since u and v are fermionic we must assume fermionic character for the coefficients c_j and d_j, while (a_j, b_j) are bosonic. Due to the fermionic character it is important to note that $c_j^2 = d_j^2 = 0$.

Now comparing the leading-order singularity leads to

$$\alpha = \beta = \gamma = \delta = -1. \tag{5}$$

Equating coefficients of terms containing ϕ^{-3} we get the following equations for the leading coefficients a_0, b_0, c_0, d_0:

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$$
\begin{aligned}
&-2\phi_x^2+k\{2(a_0^2+b_0^2)+c_0^2+d_0^2\}\\
&\quad-2k^{1/2}(c_0d_0/a_0)\phi_x=0,\\
&-2\phi_x^2+k\{2(a_0^2+b_0^2)+c_0^2+d_0^2\}\\
&\quad+k^{1/2}[(c_0^2-d_0^2)/b_0]\phi_x=0,\\
&-4\phi_x^2+k(a_0^2+b_0^2)\\
&\quad+3k^{1/2}[(a_0d_0-b_0c_0)/c_0]\phi_x=0,\\
&-4\phi_x^2+k(a_0^2+b_0^2)\\
&\quad+3k^{1/2}[(a_0c_0+b_0d_0)/d_0]\phi_x=0.
\end{aligned}
\tag{6}
$$

Remembering the condition that $c_0^2=d_0^2=0$, we see that the simplest solution to Eq. (6) is

$$
\begin{aligned}
&c_0=d_0 \quad \text{(undetermined)},\\
&b_0=0, \quad a_0=\tfrac{1}{2}.
\end{aligned}
\tag{7}
$$

Substituting in the original equation the expression for the fields,[11]

$$
\begin{aligned}
&u_0=a_0\phi^{-1}+a_r\phi^{r-1}, \quad v_0=b_0\phi^{-1}+b_r\phi^{r-1},\\
&u_1=c_0\phi^{-1}+c_r\phi^{r-1}, \quad v_1=d_0\phi^{-1}+d_r\phi^{r-1},
\end{aligned}
\tag{8}
$$

we arrive at the recurrence relation of the form

$$
\begin{aligned}
&-[b_{r-2,t}+(r-2)\phi_t b_{r-1}]\\
&\quad=[u_{r-2,xx}+\{2a_{r-1,x}(r-2)\phi_x+a_{r-1}\phi_{xx}(r-2)\}+a_r\phi_x^2(r-1)(r-2)]\\
&\quad\quad+k[2a_0(2(a_0a_r+b_0b_r)+c_0c_r+d_0d_r)+a_r\{2(a_0^2+b_0^2)\}+2a_0(a_r^2+b_r^2)\\
&\quad\quad+a_r(2[a_0a_r+b_0b_r]+c_0c_r+d_0d_r)+2a_r\{a_r^2+b_r^2\}]+k^{1/2}[(c_{0,x}d_{r-1}+d_0c_{r-1,x})+(d_{0,x}c_{r-1}+c_0d_{r-1,x})]\\
&\quad\quad+\{d_0c_r\phi_x(r-2)+c_0d_r\phi_x(r-2)\}.
\end{aligned}
\tag{9}
$$

Three other similar equations are also generated. These relations are somewhat simplified if we assume that the expansion coefficients a_j, b_j, c_j, d_j all are functions of time only. Then the condition for nonzero values of a_r, b_r, c_r, d_r leads to the vanishing of the determinant,

$$
\Delta=\begin{vmatrix}
4-r^2+3r & 0 & c_0rk^{1/2} & c_0rk^{1/2}\\
0 & -(r^2-3r) & -c_0k^{1/2}(r-2) & (r-2)c_0\\
c_0k^{1/2}(r-5) & (r-3)c_0k^{1/2} & -(2r^2-6r+3) & -(2r-3)\\
c_0k^{1/2}(r-5) & -(r-3)c_0k^{1/2} & -(2r-3) & -(2r^2-6r+3)
\end{vmatrix},
$$

which can be simplified to the form

$$
\Delta=r^2(r+1)(r-1)(r-2)(r-3)^2(r-4)=0,
\tag{10}
$$

so that the resonance positions are

$$
r=0,-1,1,2,3,4.
\tag{11}
$$

The resonance at $r=-1$ corresponds to the arbitrariness of the solution manifold $\phi(x,t)=0$. At the other resonance positions we evaluate the coefficients recursively. At $r=1$ we obtain

$$
\begin{aligned}
&a_1=0, \quad b_1=-\phi_t/2k^{1/2},\\
&d_1=\tfrac{1}{12}c_0\phi_t, \quad c_1=-\tfrac{1}{12}c_0\phi_t.
\end{aligned}
\tag{12}
$$

But since ϕ_t is not known, and also c_0, d_0 are not fixed, we see that the expansion coefficients (b_1,c_1,d_1) are arbitrary. At $r=2$, we have the complicated set of equations written below for a_2, b_2, c_2, d_2:

$$
\begin{aligned}
&6a_2+2k^{1/2}(c_2c_0+d_2c_0)\\
&\quad=-k^{1/2}[2(a_1^2+b_1^2)+4a_1^2+2c_0(c_1+d_1)],\\
&2b_2=-k^{1/2}[4a_1b_1+2c_0b_1(c_1+d_1)k^{1/2}],\\
&k^{1/2}c_0(3a_2-b_2)+c_2-d_2\\
&\quad=-d_{0t}-kc_0(a_1^2+b_1^2)-2k^{1/2}a_1c_1,\\
&k^{1/2}c_0(3a_2+b_2)-c_2+d_2\\
&\quad=c_{0t}-kd_0(a_1^2+b_1^2)-2k^{1/2}a_1d_1.
\end{aligned}
\tag{13}
$$

But since the determinant of the coefficient on the rhs of (a_2,b_2,c_2,d_2) vanishes we have really three independent equations instead of four. If we also use the above expressions for (a_1,b_1,c_1,d_1) it is easy to observe that all the coefficients (a_2,b_2,c_2,d_2) are arbitrary.

At $r=3$ all that the coefficients (a_3,b_3,c_3,d_3) are connected to the previous ones by equations of the following form:

$$
\begin{aligned}
&4a_3+3c_0k^{1/2}(c_3+d_3)\\
&\quad=-b_{1t}-b_2\phi_t-2ka_1(a_1^2+b_1^2),\\
&-c_0k^{1/2}(c_3-d_3)\\
&\quad=-a_{1t}-a_2\phi_t-2ka_1(a_1^2+b_1^2),\\
&2c_0k^{1/2}a_3-3c_3-3d_3\\
&\quad=-d_{1t}-d_2\phi_t-c_1k(a_1^2+b_1^2),\\
&2c_0k^{1/2}a_3-3c_3-3d_3\\
&\quad=c_{1t}+c_2\phi_t-kd_1(a_1^2+b_1^2).
\end{aligned}
\tag{14}
$$

So here it is evident from the last two equations of (14) that all of the coefficients (a_3,b_3,c_3,d_3) cannot be determined. Similar analyses also hold for the coefficients (a_4,b_4,c_4,d_4), so that we can conclude that the supersymmetric nonlinear Schrödinger equation is completely integrable in the sense of Painlevé test.

III. BOSONIC CASE

In our above analysis the extra nonlinear field $\psi(x,t)$ was fermionic and people have already found out the Lax pair for such system. We now want to investigate the situation when $\psi(x,t)$ is simply another bosonic field just as $q(x,t)$ and Eq. (1) is no more a super-NLSE but a new pair of coupled NLSE in ordinary variables.

Let us go back to Eqs. (6) determining the leading coef-

ficients a_0, b_0, c_0, d_0, whence this time $c_0^2 = d_0^2 \neq 0$. We deduce from (6)

$$a_0(c_0^2 - d_0^2) + 2b_0c_0d_0 = 0\,,$$
$$c_0(a_0c_0 + b_0d_0) + d_0(b_0c_0 - a_0d_0) = 0\,.$$

To solve these we assume $c_0/d_0 = x$ and $b_0/a_0 = \alpha$, so that we have the connections

$$a_0 = 4/\beta \text{ or } -1/\beta, \quad \beta^2 = 1 + \alpha^2 \tag{15}$$

and the corresponding relation between c_0 and d_0 can be written as

$$c_0 = \text{either } -d_0(\alpha + \beta) \text{ or } -d_0(\alpha - \beta)\,.$$

In the above computation we have set $\phi = x - \psi(t)$. So finally we have two distinct cases for the values of the leading coefficients:

$$\left.\begin{aligned} c_0 &= -(\alpha - \beta)d_0\,,\\ a_0 &= -4/\beta\,,\\ d_0^2 &= 12/\beta(\alpha - \beta)\,, \end{aligned}\right\} \quad \text{(A)}$$

$$\left.\begin{aligned} c_0 &= -(\alpha - \beta)d_0\,,\\ a_0 &= 1/\beta, \quad d_0^2 = 2/\beta(\alpha - \beta)\,. \end{aligned}\right\} \quad \text{(B)} \tag{16}$$

Equating coefficients of ϕ^{r-3} yields the following four equations for the coefficients (a_r, b_r, c_r, d_r):

$$a_rX + 4b_ra_0b_0k + c_r\{2a_0c_0k + d_0k^{1/2}(r-2)\phi_x\} + d_r\{2a_0d_0k + k^{1/2}c_0\phi_x(r-2)\} = 0\,, \tag{17a}$$

$$4ka_0b_0a_r + b_rY + c_r\{2b_0c_0k - k^{1/2}c_0(r-2)\phi_x\} + d_r\{2b_0d_0k + k^{1/2}d_0\phi_x(r-2)\} = 0\,, \tag{17b}$$

$$a_r\{2a_0c_0k - (r-3)k^{1/2}d_0\phi_x\} + b_r\{2b_0c_0k + k^{1/2} \times (r-3)c_0\phi_x\} + c_rZ - d_r(2r-3)a_0k^{1/2}\phi_x = 0\,, \tag{17c}$$

$$a_r\{2a_0d_0k - k^{1/2}c_0(r-3)\phi_x\} + b_r\{2b_0d_0k - d_0(r-3)k^{1/2}\phi_x\} + c_r\{-k^{1/2}(2r-3)a_0\phi_x\} + d_0T = 0\,. \tag{17d}$$

Again for nonzero values of (a_r, b_r, c_r, d_r) we set equal to zero the determinant formed by the coefficients in (17) which leads to an equation for r of the form

$$r(r-3)(r-10)(r+6)(r-5)(r+1)(r^2 - r - 60) = 0, \tag{18}$$

where

$$\begin{aligned} X &= (c_0^2 + d_0^2 + 2b_0^2 + 6a_0^2)k - (r-1)(r-2)\phi_x^2\,,\\ Y &= (6b_0^2 + 2a_0^2 + c_0^2 + d_0^2)k - (r-1)(r-2)\phi_x^2\,,\\ Z &= (a_0^2 + b_0^2)k - 2(r-1)(r-2)\phi_x^2 + (2r-3)k^{1/2}b_0\phi_x\,,\\ T &= (a_0^2 + b_0^2)k - 2(r-1)(r-2)\phi_x^2 - (2r-3)k^{1/2}b_0\phi_x\,. \end{aligned} \tag{19}$$

So the new bosonic version of our equation does have resonances at the positions

$$r = 0, -1, 3, 5, 10.$$

It is to be noted that $r = -6$ is not accessible and $r = -1$ corresponds to the arbitrariness of the wave front $\phi(x,t)$. Also the equation $r^2 - r - 60 = 0$ does not possess any integer root. In the derivation of Eqs. (18) and (19) we have considered case (A) noted previously. Case (B) can be similarly treated and the equation for the resonance positions is given by

$$\det \Delta = (8d_0/\beta)r(r-3)(r+6)(r-5) = 0\,, \tag{20}$$

so that resonance occurs only at $r = 0, 3, 5, -6$. But since the set does not contain $r = -1$, we restrict our analysis to the case (A) only in the following.[5]

IV. PROPERTIES OF EXPANSION COEFFICIENTS

To study the arbitrariness of the coefficients (a_r, b_r, c_r, d_r) at the resonance position $r = r_0$, where r_0 is a root of Eq. (18), we firstly deduce a recurrence relation for the coefficients. It can be written as

$$M = \begin{pmatrix} a_n \\ b_n \\ c_n \\ d_n \end{pmatrix} = \begin{pmatrix} \alpha_n \\ \beta_n \\ \gamma_n \\ \delta_n \end{pmatrix}, \tag{21}$$

where the matrix M and $(\alpha_n, \beta_n, \gamma_n, \delta_n)$ are given as

$$M = \begin{vmatrix} X & 4a_0b_0 & 2a_0c_0 + d_0(n-2) & 2a_0d_0 + c_0(n-2) \\ 4a_0b_0 & Y & 2b_0c_0 - c_0(n-2) & 2b_0d_0 + d_0(n-2) \\ 2a_0c_0 - (n-3)d_0 & 2b_0c_0 + (n-3)c_0 & Z & -(2n-3)a_0 \\ 2a_0d_0 - (n-3)c_0 & 2b_0d_0 - (n-3)d_0 & -(2n-3)a_0 & T \end{vmatrix},$$

$$\begin{aligned} \alpha_n &= -(n-2)b_{n-2}\phi_t - a_0\{2(a_{n-1}^2 + b_{n-1}^2) + c_{n-1}^2 + d_{n-1}^2\} - \{2a_0a_{n-1}^2 + 2b_0a_{n-1}b_{n-1}\}\,,\\ \beta_n &= -[b_0\{2(a_{n-1}^2 + b_{n-1}^2) + c_{n-1}^2 + d_{n-1}^2\}] - (n-2)a_{n-2}\phi_t\,,\\ \gamma_n &= -(n-2)d_n - 2\phi_t - c_0(a_{n-1}^2 + b_{n-1}^2)\,,\\ \delta_n &= +(n-2)c_n - 2\phi_t - d_0(a_{n-1}^2 + b_{n-1}^2)\,. \end{aligned} \tag{22}$$

Now at the resonance positions at $r = 1$,

$$d_1 = (\alpha + \beta)c_1, \quad a_1 = -\alpha b_1\,, \tag{23}$$

at $r = 2$,

$$\begin{aligned} c_2 &= -d_2(\alpha + \beta)\,, a_2 = xa_0\phi_t^2,\\ b_2 &= yb_0\phi_t^2\,, \quad c_2 = zc_0\phi_t^2, \quad d_2 = 6d_0\phi_t^2\,, \end{aligned} \tag{24}$$

which shows that the coefficients are not determined, whence (x, y, z, σ) are some numerical coefficients. In each case since the rank of the matrix on the left-hand side is always less the equations never determine the coefficients uniquely. The similar set of results can also be obtained for the coefficients at $r = 3, 5$.

V. CONCLUSION

In the above analysis we have shown that the super-NLSE is a completely integrable system and possesses the requisite Painlevé property. An important offshoot of our result is that even when the anticommuting field is considered to be commuting, the system retains the Painlevé property so that we have actually found out a new nonlinear system which is an extension of the usual NLSE which is completely integrable but whose Lax pair is still not known.

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The energy levels and the corresponding normalized wave functions for a model of a compressed atom

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In the model of a compressed atom (or ion) considered in the present paper the boundary condition associated with the corresponding uncompressed atom, i.e., the condition that the radial wave function must vanish at $r = \infty$, is replaced by the boundary condition that the radial wave function must have a node at the finite distance $r = a$. The treatment of the problem of obtaining the energy shift due to the compression is based on the phase-integral method developed by Fröman and Fröman, an essential feature of which is that one can use exact formulas in the calculations and make all approximations in the final stage. The treatment of the problem of obtaining the relative change of the wave function due to the compression is based on the rigorous evaluation of the normalization integral developed by Furry [Phys. Rev. **71**, 360 (1947)] and Yngve [J. Math. Phys. **13**, 324 (1972)], in which one also uses exact formulas in the calculations and makes all approximations in the final stage. Since compression of an atom gives rise to very subtle effects, rigorous methods are indispensible for obtaining accurate and reliable analytical final formulas. As an application, the resulting general formulas are particularized to the case of a hydrogenic atom, and a numerical illustration of the accuracy of the formulas is given.

I. INTRODUCTION

In the treatment of the radial Schrödinger equation for an atomic electron in a free, uncompressed atom (or ion) the boundary conditions are $\psi(0) = \psi(\infty) = 0$. If, however, the atom (or ion) is enclosed in a sphere of radius a, the boundary conditions are instead $\psi(0) = \psi(a) = 0$. This change of boundary condition causes a shift upwards of every energy level and an increase of the normalized wave function inside the compressed atom. These effects have been studied theoretically during several decades by many authors.[1–64]

There are a lot of physical problems that, although a boundary condition is imposed on the wave function at a surface, are not relevant for our present investigation and hence are not included in our references.[1–64] As examples of those kinds of problems we mention the following: the common model of a particle enclosed in a box, treated in textbooks on quantum mechanics, and the related model of noninteracting particles enclosed in a box, usual as a simple standard model in statistical mechanics, for instance in the electron theory of metals and in chemistry. These are models of a somewhat different nature than the model of a compressed atom considered in the present paper. So are also the models of molecular or atomic constituents with hard cores used in the theory of gases and liquids and in the calculation of phase shifts. In the cellular method of solid state physics one imposes a boundary condition on the derivative of the wave function at a finite distance from the nucleus, but this boundary condition does not cause the confinement of the system to a box and is thus of a different nature than the boundary condition used in the present paper. The latter part of this assertion is to some extent also true for the boundary condition in certain problems of surface physics when there is an atom near a rigid wall of infinite extension. In quantum chemical investigations one sometimes uses wave functions that are equal to zero outside a certain region, but again this is another kind of localization than the kind of confinement in the model of a compressed atom described above. The kinds of investigations just mentioned are not represented in our list of references,[1–64] which will now be briefly discussed.

The model of a compressed atom which we shall study in the present paper was first introduced in 1937 for the case of the hydrogen atom in a paper by Michels, de Boer, and Bijl,[1] which was soon followed by a related paper by Sommerfeld and Welker.[2] Since then problems concerning confined atoms have been studied by many authors.[3–64] The frequency of the published papers indicates a fairly constant interest in the subject over the years, except for a decrease during the sixties, which is then followed by an increased and still continuing interest.

Many papers are concerned with the hydrogenic atom, i.e., a hydrogen atom or hydrogenlike ion, in a box with impenetrable or partly penetrable walls of spherical, paraboloidal, or prolate spheroidal shape.[1,2,11,14,21,25,27,42,45,46,51–54,56] Among the subjects treated in these papers we mention calculation of shifts of energy levels,[1,46,51,54,56] polarizability,[1,51] astrophysical studies concerning planets and white dwarf stars,[2] calculation of the diamagnetic screening constant,[27] hyperfine splitting,[42,46,51,54] eigenfunctions,[51,54,56] nuclear magnetic shielding,[51] and hyperfine interaction energy.[52]

In addition to the references concerning the hydrogenic atom enumerated above, there are also some papers in which the Stark effect is treated for a hydrogenic atom confined by a spherical wall[50,58] or by paraboloidal walls.[61] In this connection we also mention papers concerning a charged parti-

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cle in a box under the influence of a uniform electric field[38,43] and possibly also a Mathieu potential[38] and papers concerning an electron or a system of electrons inside a box in a magnetic field.[17,21,34]

Another whole series of papers concerning the hydrogenic atom in a spherical box was initiated by Wigner.[22] These papers[22,24,30,36,37,39,41] are concerned with the difficulties that appear in the Rayleigh–Schrödinger perturbation theory when applied to the hydrogenic atom and are thus concerned with the applicability of perturbation theory itself. In these papers the hydrogenic atom is, in the intermediate steps of the perturbation calculation, enclosed in a spherical box of finite radius, which at the end is allowed to tend to infinity, so that the result for the usual hydrogenic atom is obtained. To this series of papers there belongs also a paper concerning the one-dimensional motion of a particle under the influence of a one-dimensional attractive delta function potential and symmetrically enclosed within infinitely high potential walls.[28] The same delta function potential model has also been considered in another paper,[59] where the purpose was, however, not to throw light on perturbation theory results.

Several papers deal with the nonrelativistic treatment of the artificially bounded harmonic oscillator, i.e., the oscillator enclosed between potential walls.[4,5,7,8,9,12,13,23,25,33,34,44,47,49,62] This kind of oscillator has also been treated relativistically.[6] The inverted linear harmonic oscillator[49] with artificial boundary conditions has also been treated. There are also papers concerning particular linear anharmonic oscillators[57,63] and particular linear, symmetric double-well oscillators[55,60] enclosed symmetrically between infinitely high potential walls. Among the physical problems treated with the model of a harmonic oscillator with artificial boundary conditions, we mention the proton–deuteron transformation as a source of energy in dense stars,[4] the fundamental mass-radius relation for a white dwarf star,[7] an investigation by Chandrasekhar[8] on the rate of escape of stars from galactic and globular clusters when allowance is made for dynamical friction, a possible role of the symmetrically bounded linear harmonic oscillator in the theory of the specific heat of solids,[12] phase transitions of second order,[13] energy levels and oscillator strengths,[23] certain anharmonic effects in solids,[33] and magnetic properties of metallic solids.[34]

Sommerfeld and Hartmann[3] have treated the problem concerning the rotation of a rigid diatomic molecule restricted to the angular region $0<\vartheta<\vartheta_0$, a problem related to ideas emanating from Pauling concerning phase transitions in certain solids as well as to Debye's theory for dipole molecules in electric fields. The same rigid rotator has also been treated with restriction to the angular region $\epsilon<\vartheta<\pi-\epsilon$.[25]

It was pointed out by ter Haar[10] that, in rigorous treatments, the boundary conditions, which were used in the papers where the Morse potential and the Rosen–Morse potential were originally introduced, should be modified from "natural" into "artificial" boundary conditions.

There are also papers concerning atoms with more than one electron[18–20] and concerning molecules[14–16,31,40,56] confined in boxes. The following topics are discussed in those references: a helium atom compressed in a spherical box,[18,19] a compressed argon atom according to a statistical model of the atom,[20] molecular physics and the virial theorem,[14] the compression of a gas composed of diatomic molecules,[15] the hydrogen molecule ion in a spheroidal box with the nuclei at the foci,[16,31] ground state energy of solid molecular hydrogen at high pressures,[40] the molecule ions H_2^+ and HeH^{++} inside spheroidal boxes with the aim of calculating energy eigenvalues and eigenfunctions, and for H_2^+ also the hyperfine splitting.[56]

Although our study of the literature to find and examine all the above-mentioned references has been rather time consuming, the papers quoted[1–64] are not claimed to constitute a complete list of relevant references. We remark, in particular, that we have come across no references to Russian papers, which may be an indication of incompleteness. For the references published after 1980 the list is expected to be less complete than for the earlier references. We have in fact not looked systematically for references from the last few years. Although our list of references[1–64] may thus not be complete, it demonstrates in any case that during almost five decades there have appeared numerous publications dealing with the model of a compressed atom discussed above. However, due to the subtlety of the effects studied and to simplifications and limitations in the various treatments, there has been no general agreement on the calculated results. Thus since reliable and accurate *analytical* formulas for the effects on energies and wave functions, due to the compression, seemed to be missing in the literature, we found it worthwhile to undertake the investigation to be described below. Our aim is to derive simple, accurate analytical results for a system consisting of a nonrelativistic quantal particle bound in an unspecified, smooth, spherically symmetric single-well potential which is enclosed in a large, impenetrable sphere.

In Sec. II the results of the method developed by Fröman and Fröman[65–67] for the rigorous solution of connection problems are described briefly but in sufficient detail to make the present paper self-contained. In Sec. III we derive an exact quantization condition for the energy levels of the above model of a compressed atom by means of the method described in Sec. II, and in Sec. IV we obtain an exact expression for the normalization integral of the corresponding wave function by means of a rigorous method devised by Furry[68] and Yngve.[69] An essential common feature of the methods applied in the present paper is that one uses exact formulas in the calculations and makes all approximations in a controllable way in the final stage. The use of such a rigorous procedure for obtaining reliable results is particularly important in the present context, since one is looking for very subtle, in fact "exponentially small," effects. It is therefore essential to have complete control of the calculations. Neglecting, in the exact quantization condition and in the exact expression for the normalization condition, certain correction quantities for which upper bounds are available, we obtain in Sec. V and Sec. VI, respectively, simple approximate formulas for the energy shift and for the relative change of the wave function due to the compression. Section VII contains a discussion of the wave function, the aim of which is to illuminate the consistency of certain results in the pres-

ent paper with results in Ref. 70. The results obtained in Secs. V and VI are in Sec. VIII generalized from the use of the first order to the use of the arbitrary-order phase-integral approximation generated from a conveniently chosen base function [see Refs. 71, 72 (pp.126–131), and 73]; see also Refs. 74–76. In Sec. IX the resulting arbitrary-order formulas are applied to the particular case of a compressed hydrogenic atom, and the accuracy of the formulas thus obtained is demonstrated graphically for the first- and third-order approximations.

II. RIGOROUS METHOD FOR THE SOLUTION OF CONNECTION PROBLEMS

In this section we give the basis for understanding the treatment in the present paper by describing in a very condensed form the method for solving connection problems, developed in Ref. 65, and by collecting results and formulas from Refs. 65–67 and 71–73 which are needed in the present paper. Some changes in notation have, however, been made. Thus $Q^2(z)$ and $Q^2_{\rm mod}(z)$ in Refs. 65–67 and 71–72 correspond to $R(r)$ and $Q^2(r)$, respectively, in the present paper. Furthermore, the definition (2.14) of the matrix $\mathbf{M}$ below differs slightly from that of the matrix $\mathbf{M}$ in Eq. (3.13) of Ref. 65.

Consider the differential equation

$$\frac{d^2\psi}{dr^2} + R(r)\psi = 0, \tag{2.1}$$

where $R(r)$ is assumed to be an analytic function of the variable r, which will be allowed to take also complex values. We introduce the two linearly independent functions

$$f_1(r) = q^{-1/2}(r)\exp[+iw(r)], \tag{2.2a}$$

$$f_2(r) = q^{-1/2}(r)\exp[-iw(r)], \tag{2.2b}$$

where

$$w(r) = \int^r q(r)dr, \tag{2.3}$$

$q(r)$ being a so far unspecified function, chosen such that the functions $f_1(r)$ and $f_2(r)$ are approximate solutions of the differential equation (2.1). By introducing convenient cuts in the complex r plane we can make $f_1(r)$ and $f_2(r)$ single valued in the region under consideration. From (2.2a), (2.2b), and (2.3) it follows that

$$f_1(r)f_2'(r) - f_2(r)f_1'(r) = -2i. \tag{2.4}$$

The method to be described below can in principle be applied for solving connection problems associated with arbitrary, linearly independent functions $f_1(r)$ and $f_2(r)$ which need not be of the form (2.2a) and (2.2b) with (2.3). A general exposition of the main features of the method, based on such unspecified functions (and in fact applied to an ordinary differential equation of arbitrary order), is given in Ref. 67. In the present paper, however, the functions $f_1(r)$ and $f_2(r)$ represent phase-integral approximations of the form (2.2a) and (2.2b) with (2.3), where the function $q(r)$ corresponding to the $(2N+1)$th-order approximation is defined by the series expansion[71–73]

$$q(r) = \sum_{n=0}^{N} Y_{2n}Q(r), \tag{2.5}$$

where $Q(r)$ is the unspecified base function from which the functions Y_{2n} are generated according to known formulas, given up to Y_{20} in Ref. 77. The first few functions Y_{2n}, which were given already in Ref. 74, are

$$Y_0 = 1, \tag{2.6a}$$

$$Y_2 = \tfrac{1}{2}\epsilon_0, \tag{2.6b}$$

$$Y_4 = -\frac{1}{8}\epsilon_0^2 - \frac{1}{8}\frac{1}{Q}\frac{d}{dr}\left(\frac{1}{Q}\frac{d\epsilon_0}{dr}\right), \tag{2.6c}$$

where

$$\epsilon_0(r) = \frac{R(r)-Q^2(r)}{Q^2(r)} + Q^{-3/2}(r)\frac{d^2}{dr^2}Q^{-1/2}(r) \tag{2.7}$$

$$= \frac{R-Q^2}{Q^2} + \frac{1}{16Q^6}\left[5\left(\frac{dQ^2}{dr}\right)^2 - 4Q^2\frac{d^2Q^2}{dr^2}\right]. \tag{2.7'}$$

In the context of the present paper, where we are dealing with the radial Schrödinger equation, we must take into account the possibility of a first- or second-order pole of $R(r)$ at $r=0$. If the conditions [cf. Eq. (11.9) in Ref. 65]

$$\lim_{r\to 0} r^2R(r) \neq \tfrac{1}{4} \tag{2.8a}$$

and [cf. Eq. (6) in Ref. 78]

$$\lim_{r\to 0} r^2[Q^2(r) - R(r)] = -\tfrac{1}{4} \tag{2.8b}$$

are fulfilled, the arbitrary-order phase-integral functions $f_1(r)$ and $f_2(r)$ remain approximate solutions of the differential equation (2.1) in the neighborhood of $r=0$. Choosing $Q(r)$ in accordance with (2.8b), we can therefore, when (2.8a) is fulfilled, in solving the connection problem start by imposing the relevant boundary condition at $r=0$. The function $-Q^2(r)$ appearing in the present paper is qualitatively depicted in Fig. 1. A possible choice of $Q^2(r)$ in accordance with (2.8b) is

$$Q^2(r) = R(r) - 1/(4r^2). \tag{2.8b'}$$

In the following exposition in this section, as well as in Secs. III–VII, we shall, for the sake of simplicity, assume that we are dealing with the first-order approximation, i.e., that according to (2.5) we have $q(r) = Q(r)$ in the expressions (2.2a), (2.2b), and (2.3). The extension from the first-order approximation to an arbitrary-order approximation is a straightforward procedure, which is described in Sec. VIII.

Any exact solution $\psi(r)$ of the differential equation (2.1), together with its derivative $\psi'(r)$, can be written

$$\psi(r) = a_1(r)f_1(r) + a_2(r)f_2(r), \tag{2.9a}$$

$$\psi'(r) = a_1(r)f_1'(r) + a_2(r)f_2'(r), \tag{2.9b}$$

$a_1(r)$ and $a_2(r)$ being uniquely determined by (2.9a) and (2.9b). Obviously, one obtains the derivative of $\psi(r)$ by differentiating (2.9a) while $a_1(r)$ and $a_2(r)$ are treated formally as if they were constants, which one achieves by imposing the condition

$$a_1'(r)f_1(r) + a_2'(r)f_2(r) = 0 \tag{2.10}$$

on the functions $a_1(r)$ and $a_2(r)$. Substituting (2.9a) into the differential equation (2.1), and using (2.10), we obtain a

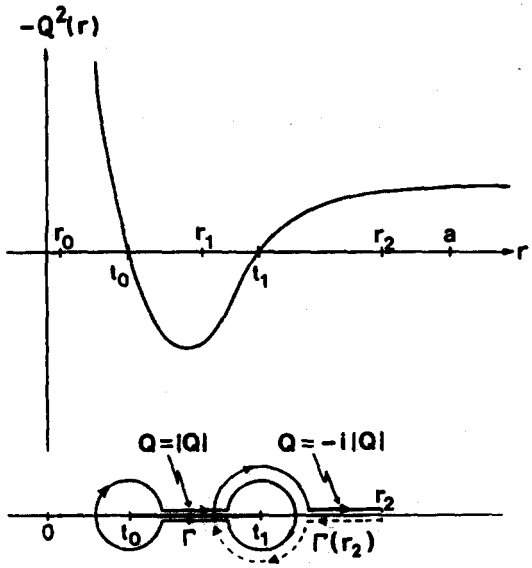

FIG. 1. For real values of r the qualitative behavior of $-Q^2(r)$ is shown. The cut in the complex r plane, introduced in order to make $Q(r)$ single valued, is indicated by a bold line, and the contours of integration occurring in the formulas are also depicted. The contour Γ is a closed loop encircling the two classical turning points t_0 and t_1. The contour $\Gamma(r_2)$ is a nonclosed contour which starts from the point on a Riemann sheet which corresponds to the point r_2 in the complex r plane under consideration, passes around the classical turning point t_1, and ends at the point r_2. The phase of $Q(r)$, which is also indicated in the figure, is chosen such that $Q(r) = |Q(r)|$ on the upper lip of the cut between t_0 and t_1.

system of two differential equations of the first order for $a_1(r)$ and $a_2(r)$, the solution of which can be obtained in closed form by means of an iteration procedure. Defining

$$\mathbf{a}(r) = \begin{pmatrix} a_1(r) \\ a_2(r) \end{pmatrix}, \tag{2.11}$$

we can describe the result as follows. Given an arbitrary column vector $\mathbf{a}(r_0)$ at the point r_0, we have for the column vector $\mathbf{a}(r)$ at the point r the following formula:

$$\mathbf{a}(r) = \mathbf{F}(r,r_0)\mathbf{a}(r_0), \tag{2.12}$$

where $\mathbf{F}(r,r_0)$ is a two-by-two matrix, the elements of which are given by convergent series; see Eqs. (3.22a)–(3.22d) and (3.3) in Ref. 65. This matrix satisfies the differential equation

$$\frac{\partial}{\partial r}\mathbf{F}(r,r_0) = \mathbf{M}(r)\mathbf{F}(r,r_0), \tag{2.13}$$

where

$$\mathbf{M}(r) = \frac{1}{2} i\epsilon_0(r)Q(r) \times \begin{pmatrix} 1 & \exp[-2i\,w(r)] \\ -\exp[2i\,w(r)] & -1 \end{pmatrix} \tag{2.14}$$

with ϵ_0 given by (2.7). The matrix $\mathbf{F}(r,r_0)$ is in fact the particular solution of the differential equation (2.13) which is equal to the two-by-two unit matrix for $r = r_0$. The following general properties of the F matrix should also be noted:

$$\mathbf{F}(r,r_0) = \mathbf{F}(r,r_1)\mathbf{F}(r_1,r_0), \tag{2.15}$$

$$\det \mathbf{F}(r,r_0) = 1, \tag{2.16}$$

$$\mathbf{F}(r,r_0) = [\mathbf{F}(r_0,r)]^{-1} = \begin{pmatrix} F_{22}(r_0,r) & -F_{12}(r_0,r) \\ -F_{21}(r_0,r) & F_{11}(r_0,r) \end{pmatrix}. \tag{2.17}$$

Useful estimates of the series defining the elements of the matrix $\mathbf{F}(r,r_0)$ can be derived on the assumption that the points r and r_0 can be connected by a path Λ in the complex r plane, on which the absolute value of $\exp[iw(r)]$ increases monotonically (or is constant) along Λ in the direction from r_0 to r. These so-called basic estimates can for our present purpose be written

$$|F_{11}(r,r_0) - 1| \leqslant \tfrac{1}{2}[\exp(\mu) - 1], \tag{2.18a}$$

$$|F_{12}(r,r_0)| \leqslant \tfrac{1}{2}[\exp(\mu) - 1]|\exp[2i\,w(r_0)]|, \tag{2.18b}$$

$$|F_{21}(r,r_0)| \leqslant \tfrac{1}{2}[\exp(\mu) - 1]|\exp[2i\,w(r)]|, \tag{2.18c}$$

$$|F_{22}(r,r_0) - 1| \leqslant \tfrac{1}{2}\mu + \tfrac{1}{2}[\exp(\mu) - 1 - \mu] \times |\exp\{2i[w(r) - w(r_0)]\}|, \tag{2.18d}$$

where μ by definition is the integral

$$\mu = \int_\Lambda |\epsilon_0(r)Q(r)dr|. \tag{2.19}$$

When using the estimates (2.18a)–(2.18d), we shall always assume that $\mu \ll 1$, which is in general the case if $R(r)$ varies slowly, if $Q^2(r)$ is chosen conveniently, and if the path Λ does not pass too close to a zero or a singularity of $Q^2(r)$.

We notice that if $\mu \ll 1$ and furthermore

$$|\exp[i\,w(r_0)]| \approx |\exp[i\,w(r)]| \approx 1,$$

the basic estimates (2.18a)–(2.18d) provide approximate values of all four elements of the matrix $\mathbf{F}(r,r_0)$, which is seen to be approximately equal to the unit matrix. On the other hand, if

$$|\exp[i\,w(r_0)]| \ll 1 \ll |\exp[i\,w(r)]|,$$

only one element, viz., $F_{11}(r,r_0)$, is determined approximately by the basic estimates (2.18a)–(2.18d). In other cases, for instance when

$$|\exp[i\,w(r_0)]| \approx 1 \ll |\exp[i\,w(r)]|,$$

the basic estimates provide approximate values of two of the elements of $\mathbf{F}(r,r_0)$. For the matrix elements, whose values are not approximately determined by the basic estimates (2.18a)–(2.18d), these estimates still give realistic orders of magnitude, i.e., the right-hand members of (2.18a)–(2.18d) although upper bounds, in general do not exceed the left-hand members very much.

More general cases, when the points r_0 and r cannot be joined by a path along which $|\exp[i\,w(r)]|$ increases monotonically, can be handled by dividing the path from r_0 to r into parts along which the absolute value of $\exp[i\,w(r)]$ is monotonic, and utilizing the multiplication rule (2.15), the inversion formula (2.17), and the basic estimates (2.18a)–(2.18d) with the notations r, r_0, and r_1 changed appropriately.

When $R(r)$ and $Q^2(r)$ are real on the real r axis, and the points r and r_0 lie on the real axis, there are certain relations between the elements of $\mathbf{F}(r,r_0)$. These so-called symmetry relations are a direct consequence of the fact that if $\psi(r)$ is a

solution of the differential equation (2.1) on the real axis, so is also the complex conjugate function $\psi^*(r)$. This fact, in turn, immediately follows from our assumption that $R(r)$ is real on the real axis.

From now on we shall assume that $R(r)$ and $Q^2(r)$ are real on the real axis and that $-Q^2(r)$ behaves, for real values of r, as indicated in Fig. 1. By restricting the variable r to lie in the upper half of the complex r plane, including the real axis with the exception of the zeros and singularities of $Q^2(r)$, we make the functions $f_1(r)$ and $f_2(r)$ single valued in the region of the complex r plane under consideration. The lower limit of integration in the definition (2.3) of $w(r)$, which has so far been unspecified, will from now on be chosen to be equal to t_0 which is the first zero of the function $Q^2(r)$ on the positive real r axis; see Fig. 1. This means that from now on $w(r)$ is defined by

$$w(r) = \int_{t_0}^{r} Q(r)dr. \tag{2.20}$$

For the case illustrated in Fig. 1 the symmetry relations for the matrix $\mathbf{F}(r_0,r_1)$ are

$$F_{12}(r_0,r_1) = iF_{11}^*(r_0,r_1), \tag{2.21a}$$

$$F_{21}(r_0,r_1) = iF_{22}^*(r_0,r_1), \tag{2.21b}$$

while those for the matrix $\mathbf{F}(r_2,r_1)$ are [cf. in Ref. 65 Eqs. (6.10a) and (6.10b) and the discussion on p. 21 of how the F matrix depends on the lower limit of integration in the definition of the w integral]

$$F_{12}(r_2,r_1) = -i\exp(-2iL)F_{11}^*(r_2,r_1), \tag{2.22a}$$

$$F_{21}(r_2,r_1) = -i\exp(+2iL)F_{22}^*(r_2,r_1), \tag{2.22b}$$

where L is defined by

$$L = \int_{t_0}^{t_1} Q(r)dr. \tag{2.23}$$

The reason why L appears in (2.22a) and (2.22b) but not in (2.21a) and (2.21b) is that $w(t_1) = L$ while $w(t_0) = 0$; see Fig. 1. The symmetry relations (2.21a), (2.21b) and (2.22a), (2.22b) are easily obtained from Eqs. (5.9a) and (5.9b) in Ref. 65 and our expression (2.20) for $w(r)$. We remark that in the limit $r_0 \to +0$ the matrix elements in (2.21a) exist and are finite, while those in (2.21b) tend to infinity; see Eqs. (4.5a)–(4.5d) in Ref. 65.

The elements of the matrix $\mathbf{F}(r_0,r_1)$ can be estimated on the assumption that the following condition is fulfilled. There exists a path Λ connecting r_0 and r_1, along which the absolute value of $\exp[i\,w(r)]$ has precisely one extremum and for which the μ integral, defined by (2.19), is much smaller than unity. This condition is in general fulfilled if r_0 and r_1 do not lie too close to the turning point t_0. In Fig. 2 it is shown qualitatively how the path Λ may proceed. We have indicated by arrows on Λ the directions in which the absolute value of $\exp[i\,w(r)]$ increases monotonically. On the real axis between t_0 and t_1, the absolute value of $\exp[i\,w(r)]$ is constant. The estimates obtained for the diagonal elements of $\mathbf{F}(r_0,r_1)$ are

$$|F_{11}(r_0,r_1) - 1| < \mu + \text{higher powers of } \mu, \tag{2.24a}$$

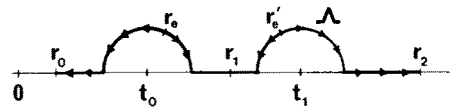

FIG. 2. How the path Λ, used to obtain the estimates (2.24a), (2.24b) and (2.26a), (2.26b), may proceed from r_0 to r_1 and from r_1 to r_2, respectively, is illustrated qualitatively. The points r_e and r_e' denote the positions of extrema for $|\exp[i\,w(r)]|$, and the directions in which this function increases monotonically are indicated by arrows.

$$|F_{22}(r_0,r_1)| < \exp[2\,|w(r_0)|] \times [\tfrac{1}{2}\mu + \text{higher powers of } \mu] \tag{2.24b}$$

if $\mu \ll 1$. According to these estimates and the symmetry relations (2.21a) and (2.21b) we thus have

$$F_{11}(r_0,r_1) \approx 1, \tag{2.25a}$$

$$F_{12}(r_0,r_1) \approx i, \tag{2.25b}$$

whereas the absolute values of the elements $F_{22}(r_0,r_1)$ and $F_{21}(r_0,r_1)$ usually become very large, since the factor $\exp[2\,|w(r_0)|]$ rapidly increases when the point r_0 moves away from the turning point t_0.

Similarly, the elements of the matrix $\mathbf{F}(r_2,r_1)$ can be estimated on a corresponding assumption; see Figs. 1 and 2. The estimates thus obtained for the diagonal elements of $\mathbf{F}(r_2,r_1)$ are

$$|F_{11}(r_2,r_1) - 1| \leqslant \mu + \text{higher powers of } \mu, \tag{2.26a}$$

$$|F_{22}(r_2,r_1)| \leqslant \exp\{2\,K(r_2)\} \times [\tfrac{1}{2}\mu + \text{higher powers of } \mu], \tag{2.26b}$$

where $\mu \ll 1$ and $K(r_2)$ is defined by

$$K(r_2) = \int_{t_1}^{r_2} iQ(r)dr = \int_{t_1}^{r_2} |Q(r)|dr. \tag{2.27}$$

Note that since the path Λ in the definition (2.19) of the μ integral is different for (2.24a), (2.24b) and (2.26a), (2.26b), μ does not denote the same quantity in (2.26a), (2.26b) as in (2.24a), (2.24b). Since $\mu \ll 1$ while in general $\frac{1}{2}\mu \exp[2\,K(r_2)] \gg 1$, we obtain from (2.26a) and (2.26b)

$$F_{11}(r_2,r_1) \approx 1, \tag{2.28a}$$

$$F_{22}(r_2,r_1) \ll \exp[2\,K(r_2)], \tag{2.28b}$$

r_2 being assumed to lie well to the right of t_1. For clarifying illustrations of the estimates discussed above, we refer to Ref. 66.

III. EXACT QUANTIZATION CONDITION

Consider the radial Schrödinger equation (2.1), i.e.,

$$\frac{d^2\psi}{dr^2} + R(r)\psi = 0, \tag{3.1}$$

where, with obvious notation,

$$R(r) = (2m/\hbar^2)[E - V(r)] - l(l+1)/r^2. \tag{3.2}$$

The boundary condition

$$\psi(0) = 0 \tag{3.3a}$$

selects a solution of the differential equation (3.1), which is unique except for an arbitrary constant factor. The further boundary condition

$$\psi(a) = 0, \tag{3.3b}$$

pertaining to the compressed atom enclosed in a sphere of radius a, yields a quantization condition. The problem of the compressed atom under consideration is thus defined by the differential equation (3.1) with (3.2) and the boundary conditions (3.3a) and (3.3b).

In atomic problems it is in general appropriate to consider the potential in which the electron moves to be real. Therefore, and also for the sake of simplicity, we restrict ourselves to assuming the potential $V(r)$ in (3.2) and hence $R(r)$, as well as the square $Q^2(r)$ of the base function $Q(r)$, introduced in connection with (2.5), to be real on the real r axis. We shall use the terminology "classically allowed" and "classically forbidden" regions (in the generalized sense) for regions where $Q^2(r)$ is positive and negative, respectively, and we shall use the term "classical turning point" or simply "turning point" (in the generalized sense) for a point where $Q^2(r) = 0$. This conforms to the terminology introduced on p. 34 in Ref. 65, although some notations used here are different, as explained in the beginning of Sec. II.

We shall start by expressing the exact solution $\psi(r)$ fulfilling the boundary condition (3.3a), i.e., $\psi(0) = 0$, in terms of the two linearly independent phase-integral functions defined by (2.2a) and (2.2b) with (2.3), where we choose $q(r)$ to be given by the first-order approximation of (2.5), i.e., $q(r) = Q(r)$. When the conditions (2.8a) and (2.8b) are fulfilled, and $Q^2(r)$ is negative for sufficiently small, positive values of r (see Fig. 1), the coefficients $a_1(r)$ and $a_2(r)$ in (2.9a) and (2.9b), corresponding to a solution $\psi(r)$ of the differential equation (3.1) fulfilling the boundary condition $\psi(0) = 0$, are given by the formulas

$$a_1(r) = F_{12}(r, +0)a_2(+0), \tag{3.4a}$$

$$a_2(r) = F_{22}(r, +0)a_2(+0). \tag{3.4b}$$

Inserting (3.4a) and (3.4b) into (2.9a) and using (2.2a) and (2.2b), we get the following expression for the exact solution $\psi(r)$ fulfilling the boundary condition (3.3a):

$$\psi(r) = (F_{12}(r, +0)\exp[2i\,w(r)] + F_{22}(r, +0))a_2(+0)f_2(r), \tag{3.5}$$

where $w(r)$ is defined by (2.3) with $q(r) = Q(r)$. Introducing now the further boundary condition (3.3b), i.e., $\psi(a) = 0$, pertaining to the compressed atom with the energy levels E_s^a, we obtain from (3.5) the quantization condition

$$F_{12}(a, +0)\exp[2i\,w(a)] + F_{22}(a, +0) = 0, \quad E = E_s^a. \tag{3.6}$$

If we let the radius a tend to infinity, the second term in the left-hand member of (3.6) becomes negligible compared to the first term, and we arrive at the quantization condition $F_{12}(+\infty, +0) = 0$ or, according to (2.17), $F_{12}(+0, +\infty) = 0$, valid for the uncompressed atom; cf. Eqs. (10.13) and (11.17) in Ref. 65. Our aim is now to bring the exact quantization condition (3.6) into a convenient form, which allows us to obtain the energy eigenvalues of the compressed atom, and to ensure that the formula we obtain for the small energy shifts, caused by the compression, yields significant results.

The qualitative behavior of the function $Q^2(r)$ for the situation we are considering is illustrated in Fig. 1. Since in the present section we use the first-order approximation, we can choose the lower limit in the integral (2.3) to be the turning point t_0 in Fig. 1, and thus we define $w(r)$ by (2.20), i.e.,

$$w(r) = \int_{t_0}^{r} Q(r)dr. \tag{3.7}$$

With the phase of $Q(r)$ chosen as indicated in Fig. 1, we obtain from (3.7), when r_2 is a point lying to the right of the turning point t_1 in Fig. 1, the formula

$$w(r_2) = L - iK(r_2), \quad r_2 > t_1, \tag{3.8}$$

where L, defined by (2.23), i.e.,

$$L = \int_{t_0}^{t_1} Q(r)dr, \tag{3.9a}$$

is a positive quantity independent of r_2 but dependent on the energy, and $K(r_2)$, defined by (2.27), i.e.,

$$K(r_2) = \int_{t_1}^{r_2} iQ(r)dr = \int_{t_1}^{r_2} |Q(r)|dr, \tag{3.9b}$$

is a positive quantity dependent on r_2 as well as on the energy.

Considering the upper half of the complex r plane, letting r_0 be a point in the classically forbidden region to the left of t_0, letting r_1 be a point in the classically allowed region between t_0 and t_1, and recalling that r_2 is a point in the classically forbidden region to the right of t_1 (see Fig. 1), we shall write in convenient forms first $F_{12}(r_2,r_0)$ and $F_{22}(r_2,r_0)$, when $r_0 = +0$ and $r = r_2$, and then the factor involving those quantities on the right-hand side of (3.5). To this purpose we use the multiplication rule (2.15) with r replaced by r_2 and the inversion formula (2.17) with r replaced by r_1, getting the identities

$$F_{12}(r_2,r_0) = -F_{11}(r_2,r_1)F_{12}(r_0,r_1) + F_{12}(r_2,r_1)F_{11}(r_0,r_1), \tag{3.10a}$$

$$F_{22}(r_2,r_0) = -F_{21}(r_2,r_1)F_{12}(r_0,r_1) + F_{22}(r_2,r_1)F_{11}(r_0,r_1). \tag{3.10b}$$

We next rewrite these identities with the aid of symmetry relations. Inserting (2.21a) and (2.22a) into (3.10a), and inserting (2.21a) and (2.22b) into (3.10b), we obtain after some rearrangements

$$\begin{aligned} F_{12}(r_2,r_0) &= -i\exp[-i(L-\tfrac{1}{2}\pi)](F_{11}(r_2,r_1) \times F_{11}^*(r_0,r_1)\exp[i(L-\tfrac{1}{2}\pi)] \\ &\quad - F_{11}^*(r_2,r_1)F_{11}(r_0,r_1)\exp[-i(L-\tfrac{1}{2}\pi)]) \\ &= 2\exp[-i(L-\tfrac{1}{2}\pi)]\,\mathrm{Im}(F_{11}(r_2,r_1) \times F_{11}^*(r_0,r_1)\exp[i(L-\tfrac{1}{2}\pi)]) \end{aligned} \tag{3.11a}$$

and

$$F_{22}(r_2,r_0) = \exp[i(L-\tfrac{1}{2}\pi)]$$
$$\times(F_{22}^*(r_2,r_1)F_{11}^*(r_0,r_1)\exp[i(L-\tfrac{1}{2}\pi)]$$
$$+F_{22}(r_2,r_1)F_{11}(r_0,r_1)\exp[-i(L-\tfrac{1}{2}\pi)])$$
$$= 2\exp[i(L-\tfrac{1}{2}\pi)]\mathrm{Im}(iF_{22}^*(r_2,r_1)$$
$$\times F_{11}^*(r_0,r_1)\exp[i(L-\tfrac{1}{2}\pi)]). \quad (3.11b)$$

With the aid of (3.8) we obtain from (3.11a):

$$F_{12}(r_2,r_0)\exp[2i\,w(r_2)]$$
$$= -2\exp[2K(r_2)]\exp[i(L-\pi/2)]\mathrm{Im}(F_{11}(r_2,r_1)$$
$$\times F_{11}^*(r_0,r_1)\exp[i(L-\pi/2)]). \quad (3.12)$$

We shall now rewrite (3.11b) into a more convenient form. To this purpose we note that, by means of the symmetry relations (2.22a) and (2.22b), the relation (2.16) yielded by the determinant of the matrix $\mathbf{F}(r_2,r_1)$ can be written as follows [cf. Eq. (6.11) in Ref. 65]

$$\mathrm{Re}(F_{11}^*(r_2,r_1)F_{22}^*(r_2,r_1)) = \tfrac{1}{2}. \quad (3.13)$$

Therefore

$$F_{11}^*(r_2,r_1)F_{22}^*(r_2,r_1) = \tfrac{1}{2} + i\,\mathrm{Im}[F_{11}^*(r_2,r_1)F_{22}^*(r_2,r_1)] \quad (3.14)$$

and hence

$$iF_{22}^*(r_2,r_1) = F_{11}(r_2,r_1)\left(\frac{i}{2|F_{11}(r_2,r_1)|^2} - \mathrm{Im}\frac{F_{22}^*(r_2,r_1)}{F_{11}(r_2,r_1)}\right). \quad (3.15)$$

Inserting (3.15) into (3.11b), we obtain

$$F_{22}(r_2,r_0) = -2\exp[2K(r_2)]\exp[i(L-\pi/2)]$$
$$\times\mathrm{Im}[F_{11}(r_2,r_1)F_{11}^*(r_0,r_1)$$
$$\times\exp[i(L-\tfrac{1}{2}\pi)](\delta_2(r_2,r_1) - i\delta_1(r_2,r_1))], \quad (3.12')$$

where

$$\delta_1(r_2,r_1) = \tfrac{1}{2}\exp[-2K(r_2)]/|F_{11}(r_2,r_1)|^2, \quad (3.16a)$$

$$\delta_2(r_2,r_1) = \mathrm{Im}(F_{22}^*(r_2,r_1)\exp[-2K(r_2)]/F_{11}(r_2,r_1)). \quad (3.16b)$$

Adding (3.12a) and (3.12b), we obtain

$$F_{12}(r_2,r_0)\exp[2i\,w(r_2)] + F_{22}(r_2,r_0)$$
$$= -2\exp[2K(r_2)]\exp[i(L-\tfrac{1}{2}\pi)]$$
$$\times\mathrm{Im}([(1+\delta_2) - i\delta_1]F_{11}^*(r_0,r_1)F_{11}(r_2,r_1)$$
$$\times\exp[i(L-\tfrac{1}{2}\pi)]). \quad (3.17)$$

Since the conditions (2.8a) and (2.8b) are assumed to be fulfilled, and since $Q^2(r)$ is negative for sufficiently small positive values of r, the relation (3.17) with (3.16a) and (3.16b) remains valid when $r_0 \to +0$, since all F matrix elements appearing in these formulas remain finite and well defined when $r_0 \to +0$; see Chap. 4 in Ref. 65. Putting $r_0 = +0$, we thus obtain from (3.17):

$$F_{12}(r_2,+0)\exp[2i\,w(r_2)] + F_{22}(r_2,+0)$$
$$= -2\exp[2K(r_2)]$$
$$\times\exp[i(L-\tfrac{1}{2}\pi)]|F_{11}(+0,r_1)F_{11}(r_2,r_1)|$$
$$\times([1+\delta_2(r_2,r_1)]^2 + [\delta_1(r_2,r_1)]^2)^{1/2}$$
$$\times\sin[\mathscr{L}(r_2,E) - \pi/2], \quad (3.18)$$

where

$$\mathscr{L}(r_2,E) = L + \arg\frac{F_{11}(r_2,r_1)}{F_{11}(+0,r_1)} - \arctan\frac{\delta_1(r_2,r_1)}{1+\delta_2(r_2,r_1)}. \quad (3.19)$$

It should be noted that all formulas (3.10)–(3.15) and (3.17)–(3.18) are identities and thus valid for any value of the energy.

For later use we shall now give some formulas for the quantity defined by (3.19). From the definitions (3.16a) and (3.16b), the estimates (2.28a) and (2.28b), and the fact that $\exp[-2K(r_2)]$ tends to zero as $r_2 \to +\infty$ it follows that $\delta_2(r_2,r_1)$ is small compared to unity and that $\delta_1(r_2,r_1)$ tends to zero as $r_2 \to +\infty$. From (3.19) it therefore follows that

$$\mathscr{L}(\infty,E) = L + \arg[F_{11}(+\infty,r_1)/F_{11}(+0,r_1)]. \quad (3.20)$$

Using (2.13)–(2.15) and (2.17), we find that

$$\frac{d}{dr}\frac{F_{11}(+\infty,r)}{F_{11}(+0,r)}$$
$$= \frac{d}{dr}\frac{F_{22}(r,+\infty)}{F_{22}(r,+0)}$$
$$= F_{12}(+0,+\infty)\frac{\epsilon_0(r)Q(r)\exp[2i\,w(r)]}{2i[F_{11}(+0,r)]^2}. \quad (3.21)$$

Recalling that the quantization condition for the uncompressed atom is $F_{12}(+0,+\infty) = 0$ [cf. Eqs. (10.13) and (11.17) in Ref. 65], we conclude from (3.21) that the quantity $F_{11}(+\infty,r)/F_{11}(+0,r)$ varies rapidly with r unless E is an eigenvalue of the uncompressed atom. With the aid of (3.20) we can rewrite (3.19) as follows:

$$\mathscr{L}(r_2,E) = \mathscr{L}(\infty,E) - \left(\arctan\frac{\delta_1(r_2,r_1)}{1+\delta_2(r_2,r_1)} - \arg\frac{F_{11}(r_2,r_1)}{F_{11}(+\infty,r_1)}\right), \quad (3.22)$$

and hence we obtain

$$\mathscr{L}(a,E) = \mathscr{L}(\infty,E) - \left(\arctan\frac{\delta_1(a,r_1)}{1+\delta_2(a,r_1)} - \arg\frac{F_{11}(a,r_1)}{F_{11}(+\infty,r_1)}\right) \quad (3.23)$$

and

$$\mathscr{L}(r_2,E) = \mathscr{L}(a,E) - \left(\arctan\frac{\delta_1(r_2,r_1)}{1+\delta_2(r_2,r_1)} - \arg\frac{F_{11}(r_2,r_1)}{F_{11}(+\infty,r_1)}\right)$$
$$+\left(\arctan\frac{\delta_1(a,r_1)}{1+\delta_2(a,r_1)} - \arg\frac{F_{11}(a,r_1)}{F_{11}(+\infty,r_1)}\right). \quad (3.24)$$

As we shall see in Sec. V, the factors multiplying the sine in (3.18) are all different from zero when r_2 lies well to the right of t_1. If the point a also fulfills that condition, the quantization condition (3.6) is thus equivalent to

$$\sin[\mathscr{L}(a,E)-\pi/2]=0, \quad E=E_s^a. \tag{3.25}$$

Therefore the exact quantization condition for the compressed atom is

$$\mathscr{L}(a,E_s^a)=(s+\tfrac{1}{2})\pi, \tag{3.26}$$

where s is an integer, which is non-negative, since the dominating term in the expression (3.19) for $\mathscr{L}(r_2,E)$, when E is an eigenvalue, is the positive term L. The exact quantization condition for the uncompressed atom is

$$\mathscr{L}(\infty,E_s^\infty)=(s+\tfrac{1}{2})\pi. \tag{3.27}$$

Subtracting (3.27) from (3.26) and using (3.23), we obtain

$$\mathscr{L}(\infty,E_s^a)-\mathscr{L}(\infty,E_s^\infty)=\left(\arctan\frac{\delta_1(a,r_1)}{1+\delta_2(a,r_1)}-\arg\frac{F_{11}(a,r_1)}{F_{11}(+\infty,r_1)}\right)_{E=E_s^a}. \tag{3.28}$$

This is a convenient exact relation from which an approximate analytic expression for the energy shift will be derived in Sec. V.

IV. EXACT FORMULA FOR THE NORMALIZATION INTEGRAL

We shall now assume that the function $R(r)$ in the differential equation (2.1) depends on a parameter E, which can for the moment be left unspecified. Let $\psi(r)$ and $\bar{\psi}(r)$ be solutions of the differential equation such that

$$\psi(0)=0 \quad \text{for every } E, \tag{4.1}$$

$$\bar{\psi}(a)=0 \quad \text{for every } E, \tag{4.2}$$

and

$$\psi(r)=\bar{\psi}(r) \quad \text{for } E=E_s^a, \tag{4.3}$$

E_s^a being an eigenvalue of the differential equation for the interval $(0,a)$; see (3.3a) and (3.3b). Under these assumptions one obtains from the work by Furry[68] and Yngve[69] the formula

$$\int_0^a\left(\frac{\partial R(r)}{\partial E}[\psi(r)]^2\right)_{E=E_s^a}dr=\left(\frac{dW(E)}{dE}\right)_{E=E_s^a}, \tag{4.4}$$

where $W(E)$ is the Wronskian

$$W(E)=\psi(r)\bar{\psi}'(r)-\bar{\psi}(r)\psi'(r), \tag{4.5}$$

a prime denoting differentiation with respect to r. In the particular case when $R(r)$ is given by (3.2), formula (4.4) simplifies to a formula for the normalization integral:

$$\int_0^a[\psi(r,E_s^a)]^2\,dr=\frac{\hbar^2}{2m}\left(\frac{dW}{dE}\right)_{E=E_s^a}. \tag{4.6}$$

The wave function $\psi(r)$, which fulfills the boundary condition (4.1), and its derivative $\psi'(r)$ are given by (2.9a) and (2.9b) with $f_1(r)$, $f_2(r)$ given by (2.2a), (2.2b), and (2.3), and $a_1(r)$, $a_2(r)$ given by (3.4a) and (3.4b). Similarly the wave function $\bar{\psi}(r)$, fulfilling the boundary condition (4.2), and its derivative $\bar{\psi}'(r)$ are given by

$$\bar{\psi}(r)=\bar{a}_1(r)f_1(r)+\bar{a}_2(r)f_2(r), \tag{4.7a}$$

$$\bar{\psi}'(r)=\bar{a}_1(r)f_1'(r)+\bar{a}_2(r)f_2'(r), \tag{4.7b}$$

where the condition $(a<\infty)$

$$\bar{a}_2(a)=-[f_1(a)/f_2(a)]\bar{a}_1(a)=-\exp[2i\,w(a)]\bar{a}_1(a) \tag{4.8}$$

must be fulfilled because of the requirement (4.2) and the definitions (2.2a) and (2.2b).

We shall now evaluate the Wronskian (4.5) of $\psi(r)$ and $\bar{\psi}(r)$. Inserting (2.9a), (2.9b), and (4.7a), (4.7b) into (4.5), we obtain the formula

$$W=(a_1\bar{a}_2-a_2\bar{a}_1)(f_1f_2'-f_2f_1'), \tag{4.9}$$

which, with the aid of (2.4), can be written

$$W=-2i(a_1\bar{a}_2-a_2\bar{a}_1). \tag{4.10}$$

It is well known that the Wronskian W is independent of r, and we can therefore evaluate it for $r=a$. Inserting thus (3.4a) and (3.4b) with $r=a$ and (4.8) into (4.10), we obtain

$$W=2i(F_{12}(a,+0)\exp[2i\,w(a)]+F_{22}(a,+0))a_2(+0)\bar{a}_1(a). \tag{4.11}$$

The requirement (4.3) implies that

$$a_1(a)=\bar{a}_1(a) \quad \text{for } E=E_s^a, \tag{4.12}$$

which combined with (3.4a) yields

$$\bar{a}_1(a)=F_{12}(a,+0)a_2(+0) \quad \text{for } E=E_s^a. \tag{4.13}$$

Using (4.11) and (4.13), and recalling the quantization condition (3.6), we obtain from (4.6)

$$\int_0^a[\psi(r;E_s^a)]^2\,dr=i\frac{\hbar^2}{m}\left[[a_2(+0)]^2F_{12}(a,+0)\frac{\partial}{\partial E}(F_{12}(a,+0)\times\exp[2i\,w(a)]+F_{22}(a,+0))\right]_{E=E_s^a}. \tag{4.14}$$

Inserting (3.18) with $r_2=a$ into (4.14), and recalling that the eigenvalues E_s^a must fulfill the quantization condition (3.25), we obtain

$$\int_0^a[\psi(r;E_s^a)]^2\,dr=-\frac{2i\,\hbar^2}{m}\left[[a_2(+0)]^2\exp[2K(a)]\times\exp[i(L-\pi/2]F_{12}(a,+0)|F_{11}(+0,r_1)\times F_{11}(a,r_1)|([1+\delta_2(a,r_1)]^2+[\delta_1(a,r_1)]^2)^{1/2}\times\frac{\partial}{\partial E}\sin\left[\mathscr{L}(a,E)-\frac{\pi}{2}\right]\right]_{E=E_s^a}. \tag{4.15}$$

From (3.11a) with $r_0=+0$ and $r_2=a$ we obtain

$$F_{12}(a,+0)=2\exp[-i(L-\pi/2)]|F_{11}(a,r_1)F_{11}(+0,r_1)|\times\sin\left(L-\frac{\pi}{2}+\arg\frac{F_{11}(a,r_1)}{F_{11}(+0,r_1)}\right). \tag{4.16}$$

With the aid of (3.19), (3.26), and (3.16a) we obtain from (4.16) when $E=E_s^a$

$$F_{12}(a,+0) = 2\exp[-i(L-\pi/2)]|F_{11}(a,r_1)F_{11}(+0,r_1)|\sin\left(\mathscr{L}(a,E_s^a) - \frac{\pi}{2} + \arctan\frac{\delta_1(a,r_1)}{1+\delta_2(a,r_1)}\right)$$

$$= 2\exp[-i(L-\pi/2)]|F_{11}(a,r_1)F_{11}(+0,r_1)|\sin\left(s\pi + \arctan\frac{\delta_1(a,r_1)}{1+\delta_2(a,r_1)}\right)$$

$$= 2\exp[-i(L-\pi/2)]|F_{11}(a,r_1)F_{11}(+0,r_1)|(-1)^s\frac{\delta_1(a,r_1)}{\{[1+\delta_2(a,r_1)]^2+[\delta_1(a,r_1)]^2\}^{1/2}}$$

$$= (-1)^s\frac{\exp[-i(L-\pi/2)]\exp[-2K(a)]|F_{11}(+0,r_1)|}{|F_{11}(a,r_1)|\{[1+\delta_2(a,r_1)]^2+[\delta_1(a,r_1)]^2\}^{1/2}}, \quad E = E_s^a. \tag{4.17}$$

Inserting (4.17) into (4.15) and using the exact quantization condition (3.26), we obtain

$$\int_0^a [\psi(r;E_s^a)]^2\,dr = \frac{2\hbar^2}{m}\left(\left[a_2(+0)\exp\left(-\frac{1}{4}\pi i\right)\right]^2|F_{11}(+0,r_1)|^2\frac{\partial\mathscr{L}(a,E)}{\partial E}\right)_{E=E_s^a}. \tag{4.18}$$

For the uncompressed atom, i.e., for $a=\infty$, we obtain from (4.18)

$$\int_0^\infty [\psi(r;E_s^\infty)]^2\,dr = \frac{2\hbar^2}{m}\left(\left[a_2(+0)\exp\left(-\frac{1}{4}\pi i\right)\right]^2|F_{11}(+0,r_1)|^2\frac{\partial\mathscr{L}(\infty,E)}{\partial E}\right)_{E=E_s^\infty}. \tag{4.19}$$

Introducing the normalization conditions

$$\int_0^a [\psi(r;E_s^a)]^2\,dr = \int_0^\infty [\psi(r,E_s^\infty)]^2\,dr = 1, \tag{4.20}$$

we obtain from (4.18) and (4.19) the exact formula

$$\frac{[a_2(+0;E_s^a)]^2 - [a_2(+0;E_s^\infty)]^2}{[a_2(+0;E_s^a)]^2}$$

$$= \frac{1/[a_2(+0;E_s^\infty)]^2 - 1/[a_2(+0;E_s^a)]^2}{1/[a_2(+0;E_s^\infty)]^2}$$

$$= \frac{(|F_{11}(+0,r_1)|^2\,\partial\mathscr{L}(\infty,E)/\partial E)_{E=E_s^\infty} - (|F_{11}(+0,r_1)|^2\partial\mathscr{L}(a,E)/\partial E)_{E=E_s^a}}{(|F_{11}(+0,r_1)|^2\,\partial\mathscr{L}(\infty,E)/\partial E)_{E=E_s^\infty}} \tag{4.21}$$

for the relative change of the square of the normalization factor of the wave function, due to the compression of the atom.

V. DERIVATION OF APPROXIMATE FORMULAS FOR THE ENERGY SHIFT DUE TO THE COMPRESSION OF THE ATOM

We shall first derive a sufficiently sharp estimate for the last term on the right-hand side of (3.22). Using (2.13), (2.14), (2.22b), (3.8), (3.15), and the definitions (3.16a) and (3.16b), we obtain

$$\frac{\partial}{\partial r_2}F_{11}(r_2,r_1)$$

$$= M_{11}(r_2)F_{11}(r_2,r_1) + M_{12}(r_2)F_{21}(r_2,r_1)$$

$$= \tfrac{1}{2}iQ(r_2)\epsilon_0(r_2)(F_{11}(r_2,r_1)$$

$$+ \exp[-2i\,w(r_2)]F_{21}(r_2,r_1))$$

$$= \tfrac{1}{2}iQ(r_2)\epsilon_0(r_2)F_{11}(r_2,r_1)(1 - i\exp[-2K(r_2)]$$

$$\times F_{22}^*(r_2,r_1)/F_{11}(r_2,r_1))$$

$$= \tfrac{1}{2}iQ(r_2)\epsilon_0(r_2)F_{11}(r_2,r_1)$$

$$\times(1+\delta_2(r_2,r_1) - i\delta_1(r_2,r_1)),$$

i.e.,

$$\frac{\partial}{\partial r_2}\ln F_{11}(r_2,r_1)$$

$$= \tfrac{1}{2}iQ(r_2)\epsilon_0(r_2)(1+\delta_2(r_2,r_1) - i\delta_1(r_2,r_1)). \tag{5.1}$$

From (5.1) it follows that

$$\ln F_{11}(+\infty,r_1) - \ln F_{11}(r_2,r_1)$$

$$= \int_{r_2}^\infty \frac{1}{2}iQ(r_2)\epsilon_0(r_2)(1+\delta_2(r_2,r_1) - i\delta_1(r_2,r_1))dr_2. \tag{5.2}$$

In the integrand of (5.2), $\delta_1(r_2,r_1)$ and $iQ(r_2)$ are positive, and $\epsilon_0(r_2)$ and $\delta_2(r_2,r_1)$ are real. Hence, taking the imaginary part of (5.2), we obtain

$$\arg\frac{F_{11}(r_2,r_1)}{F_{11}(+\infty,r_1)} = \int_{r_2}^\infty \frac{1}{2}|Q(r_2)|\epsilon_0(r_2)\delta_1(r_2,r_1)dr_2. \tag{5.3}$$

Using the definitions (3.16a) and (3.9b) and the estimate (2.26a), we obtain from (5.3) the estimate

$$\left|\arg\frac{F_{11}(r_2,r_1)}{F_{11}(+\infty,r_1)}\right|$$

$$< \exp[-2K(r_2)]$$

$$\times\int_{r_2}^\infty |\epsilon_0(r_2)Q(r_2)|dr_2 \ll \exp[-2K(r_2)]. \tag{5.4}$$

For a discussion of the smallness of the μ integral in the second member of (5.4) [cf. (2.19)] we refer to Refs. 65 and 66. *The result* (5.4) *is a crucial estimate that makes it possible to neglect the second term in the right-hand member of (3.28),* as will be demonstrated below.

From the definitions (3.16a), (3.16b) and the estimates (2.26a) and (2.26b) it follows that $\delta_1(r_2,r_1)$ is approximately equal to $\exp[-2K(r_2)]/2$ and that $\delta_2(r_2,r_1)$ is much smaller than unity. Thus we have

$$\arctan\frac{\delta_1(r_2,r_1)}{1+\delta_2(r_2,r_1)}\approx\frac{1}{2}\exp[-2K(r_2)]\,. \tag{5.5}$$

By means of (5.4) and (5.5) with $r_2=a$ we obtain from (3.28) the approximate formula

$$\mathscr{L}(\infty,E_s^a)-\mathscr{L}(\infty,E_s^\infty)\approx\tfrac{1}{2}\exp[-2K(a)]\,, \tag{5.6}$$

where, because of the approximations introduced, it is appropriate to evaluate $K(a)$ for $E=E_s^\infty$.

Since the difference $E_s^a-E_s^\infty$ is very small, we can replace the left-hand member of (5.6) by the first term in its Taylor series, getting

$$\left[\frac{\partial\mathscr{L}(\infty,E)}{\partial E}\right]_{E=E_s^\infty}(E_s^a-E_s^\infty)\approx\frac{1}{2}\exp[-2K(a)]\,. \tag{5.7}$$

Considering the quantum number s as a continuous variable, we obtain from the quantization condition (3.27) the approximate formula

$$\left[\frac{\partial\mathscr{L}(\infty,E)}{\partial E}\right]_{E=E_s^\infty}=\frac{\pi}{dE_s^\infty/ds} \tag{5.8}$$

by means of which we obtain from (5.7) the approximate formula

$$E_s^a-E_s^\infty\approx\frac{1}{2\pi}\frac{dE_s^\infty}{ds}(\exp[-2K(a)])_{E=E_s^\infty}. \tag{5.9}$$

The quantity dE_s^∞/ds can be obtained from spectroscopic data for an actual uncompressed atom or from calculated values of E_s^∞ for a model of the uncompressed atom.

We shall now derive an alternative approximate formula for $E_s^a-E_s^\infty$ by evaluating the left-hand member of (5.6) in another approximate way. For the bound states, L is at least of the order of unity, while the absolute values of $F_{11}(+0,r_1)-1$ and $F_{11}(+\infty,r_1)-1$ are much smaller than unity according to the estimates (2.24a) and (2.26a) with $r_0=+0$ and $r_2=+\infty$. Hence the absolute value of $\arg[F_{11}(+\infty,r_1)/F_{11}(+0,r_1)]$ is much smaller than L. It is reasonable to assume that the same is true for the energy derivatives of these two quantities, and therefore the energy derivative of $L+\arg[F_{11}(+\infty,r_1)/F_{11}(+0,r_1)]$ is approximately equal to the energy derivative of L. One can also express this by saying that $\arg[F_{11}(+\infty,r_1)/F_{11}(+0,r_1)]$ changes much more slowly than L when the energy changes. From (3.20) it therefore follows that the expression in the left-hand member of (5.6) can be approximately replaced by $L(E_s^a)-L(E_s^\infty)$. Thus we obtain

$$L(E_s^a)-L(E_s^\infty)\approx\tfrac{1}{2}\exp[-2K(a)]_{E=E_s^\infty}. \tag{5.10}$$

Approximating the left-hand member of (5.10) by the first term in its Taylor series, we obtain

$$E_s^a-E_s^\infty=\left(\frac{\exp[-2K(a)]}{2\,\partial L/\partial E}\right)_{E=E_s^\infty}. \tag{5.11}$$

Assuming that $Q^2(r)-R(r)$ is independent of E, we obtain from (3.9a) and (3.2)

$$\left[\frac{\partial L}{\partial E}\right]_{E=E_s^\infty}=\frac{m}{\hbar^2}\int_{t_0}^{t_1}\frac{dr}{Q(r,E_s^\infty)}. \tag{5.12}$$

We remark that when $Q^2(r)$ is equal to $R(r)$, the quantity in the right-hand member of (5.12) is equal to $T/(2\hbar)$, where T is the time for a complete classical oscillation forth and back in the radial potential well. Inserting (5.12) into (5.11), we obtain

$$E_s^a-E_s^\infty\approx\frac{\hbar^2}{2m}\left(\frac{\exp[-2K(a)]}{\int_{t_0}^{t_1}Q^{-1}(r)dr}\right)_{E=E_s^\infty}. \tag{5.13}$$

The denominator in (5.13) can be calculated when the physical potential $V(r)$ is assumed to be known, and a convenient expression for $Q^2(r)-R(r)$ is used; see (3.2).

The generalization to phase-integral approximations of arbitrary order will be considered in Sec. VIII of the present paper. However, we remark already at this point that the use of higher-order phase-integral approximations in (5.9) changes only the expression for $K(a)$, while in (5.13) also the denominator in the right-hand member changes.

VI. DERIVATION OF AN APPROXIMATE FORMULA FOR THE RELATIVE CHANGE OF THE NORMALIZED WAVE FUNCTION, DUE TO THE COMPRESSION OF THE ATOM

According to (2.24a) we have the estimate

$$F_{11}(+0,r_1)=1+O(\mu) \tag{6.1}$$

and hence

$$|F_{11}(+0,r_1)|^2\frac{\partial\mathscr{L}(a,E)}{\partial E}=\frac{\partial\mathscr{L}(a,E)}{\partial E}+O(\mu)\frac{\partial\mathscr{L}(a,E)}{\partial E}. \tag{6.2}$$

In the right-hand member of (6.2) the term $O(\mu)\,\partial\mathscr{L}(a,E)/\partial E$ is much smaller than the term $\partial\mathscr{L}(a,E)/\partial E$, and therefore $O(\mu)\,\partial\mathscr{L}(a,E)/\partial E$ should change much more slowly than $\partial\mathscr{L}(a,E)/\partial E$ when the radius a and the energy E change, unless strange cancellations occur. Therefore we obtain from (4.21) the approximate formula

$$\frac{[a_2(+0,E_s^a)]^2-[a_2(+0,E_s^\infty)]^2}{[a_2(+0,E_s^a)]^2}\approx\frac{[\partial\mathscr{L}(\infty,E)/\partial E]_{E=E_s^\infty}-[\partial\mathscr{L}(a,E)/\partial E]_{E=E_s^a}}{[\partial\mathscr{L}(\infty,E)/\partial E]_{E=E_s^\infty}}. \tag{6.3}$$

From the quantization condition (3.26) one obtains the approximate formula

$$\left(\frac{\partial\mathscr{L}(a,E)}{\partial E}\right)_{E=E_s^a}=\frac{\pi}{dE_s^a/ds},\quad a<\infty, \tag{6.4}$$

with the aid of which (6.3) gives the approximate formula

$$\frac{[a_2(+0;E_s^a)]^2-[a_2(+0;E_s^\infty)]^2}{[a_2(+0;E_s^a)]^2}=1-\frac{dE_s^\infty/ds}{dE_s^a/ds}. \tag{6.5}$$

Putting

$$a_2(+0,E_s^a)+a_2(+0,E_s^\infty)\approx 2a_2(+0,E_s^a)\,, \tag{6.6}$$

we obtain from (6.5) the approximate formula

$$\frac{a_2(+0;E_s^a)-a_2(+0;E_s^\infty)}{a_2(+0;E_s^a)}=\frac{1}{2}\left(1-\frac{dE_s^\infty/ds}{dE_s^a/ds}\right). \tag{6.7}$$

This simple formula for the relative change of the normalized wave function, due to the compression of the atom, is not quite unexpected, in view of the known formula for the normalization factor of an atom; see Eq. (24) in Ref. 79.

VII. DISCUSSION OF APPROXIMATE EXPRESSIONS FOR THE WAVE FUNCTION OF THE COMPRESSED ATOM

For the purpose of the investigation in the present paper it is not necessary to have approximate expressions for the wave function $\psi(r)$ in the intervals $0\leqslant r<t_0$, $t_0<r<t_1$, and $t_1<r\leqslant a$, but it is instructive to discuss the effect of the compression of the atom on the approximate expressions for the wave function in these intervals.

By means of the inversion formula (2.17) and the basic estimates (2.18a) and (2.18b) we obtain from (3.5) the approximate formula

$$\psi(r)\approx a_2(+0)f_2(r_0),\quad 0\leqslant r_0<t_0. \tag{7.1}$$

The wave function in the interval $t_0<r_1<t_1$ can then be obtained by means of the connection formula which is given by Eq. (8.21) in Ref. 65. The result can be written

$$\psi(r_1)\approx a_2(+0)\exp(-i\pi/4)(\exp(-i\pi/4)f_1(r_1) + \exp(+i\pi/4)f_2(r_1)),\quad t_0<r_1<t_1. \tag{7.2}$$

We shall now consider the wave function in the interval $t_1<r_2\leqslant a$. For $E=E_s^a$ we obtain from (3.18), (3.24), and (3.26)

$$\begin{aligned}&F_{12}(r_2,+0)\exp[2iw(r_2)]+F_{22}(r_2,+0)\\&\quad=2\exp[2K(r_2)]\exp\{i[L-(s+\tfrac{1}{2})\pi]\}\\&\qquad\times|F_{11}(+0,r_1)F_{11}(r_2,r_1)|\\&\qquad\times([1+\delta_2(r_2,r_1)]^2+[\delta_1(r_2,r_1)]^2)^{1/2}\\&\qquad\times\sin\left[\left(\arctan\frac{\delta_1(r_2,r_1)}{1+\delta_2(r_2,r_1)}\right)-\arg\frac{F_{11}(r_2,r_1)}{F_{11}(+\infty,r_1)}\right.\\&\qquad\left.-\left(\arctan\frac{\delta_1(a,r_1)}{1+\delta_2(a,r_1)}-\arg\frac{F_{11}(a,r_1)}{F_{11}(+\infty,r_1)}\right)\right],\\&\quad E=E_s^a.\end{aligned} \tag{7.3}$$

When $\exp[-2K(a)]\ll 1$ we obtain from (3.19), (3.26), (5.5), (2.24a), and (2.26a)

$$L\approx(s+\tfrac{1}{2})\pi,\quad E=E_s^a, \tag{7.4}$$

and when $\exp[-2K(r_2)]\ll 1$ we obtain from (3.16a), (3.16b) and (2.26a), (2.26b)

$$([1+\delta_2(r_2,r_1)]^2+[\delta_1(r_2,r_1)]^2)^{1/2}\approx 1. \tag{7.5}$$

Using (7.4), (7.5), (2.24a), (2.26a), (5.4), and (5.5), we obtain from (7.3) the approximate formula

$$\begin{aligned}&F_{12}(r_2,+0)\exp[2iw(r_2)]+F_{22}(r_2,+0)\\&\quad\approx 2\exp[2K(r_2)]\sin(\tfrac{1}{2}\exp[-2K(r_2)]\\&\qquad-\tfrac{1}{2}\exp[-2K(a)])\\&\quad\approx\exp[2K(r_2)](\exp[-2K(r_2)]-\exp[-2K(a)])\\&\quad=1-\exp\{-2[K(a)-K(r_2)]\},\\&\qquad t_1<r_2\leqslant a,\quad \exp[-2K(r_2)]\ll 1,\quad E=E_s^a.\end{aligned} \tag{7.6}$$

Inserting (7.6) into (3.5) with r replaced by r_2, we get

$$\psi(r_2)\approx(1-\exp\{-2[K(a)-K(r_2)]\})a_2(+0)f_2(r_2),\quad t_1<r_2\leqslant a,\quad \exp[-2K(r_2)]\ll 1,\quad E=E_s^a. \tag{7.7}$$

In the last member of (7.6) and in (7.7) the quantity $\exp\{-2[K(a)-K(r_2)]\}$ is significant compared to unity only as long as r_2 does not move away too far from a. Hence, when the point r_2 lies sufficiently far away from the point a, one should replace (7.7) by

$$\psi(r_2)\approx a_2(+0)f_2(r_2),\quad t_1<r_2<a,\quad \exp[-2K(a)]\ll\exp[-2K(r_2)]\ll 1,\quad E=E_s^a. \tag{7.8}$$

From (7.1), (7.2), (7.7), and (7.8) we see that the compression of the atom affects not only the energy and the normalization factor but also the analytic form of the phase-integral expression for the wave function in the part of the interval $t_1<r\leqslant a$, where $\exp[2K(r)-2K(a)]$ is not too small compared to unity. We also remark that the formulas (7.1) and (7.8) are in agreement with the result that for an uncompressed atom $\psi(r)\approx a_2(+0)f_2(r)$ for $E=E_s^\infty$ when r lies well to the left of t_0 as well as when r lies well to the right of t_1; see Ref. 70.

VIII. GENERALIZATION TO APPROXIMATIONS OF ARBITRARY ORDER

We assume that the function $R(r)$ in the differential equation (3.1) fulfills the condition (2.8a) and that the base function $Q(r)$ is chosen in agreement with the condition (2.8b). The arbitrary-order phase-integral approximation, obtained from (2.2a), (2.2b), (2.3), (2.5), (2.6a)–(2.6c) [for $2N+1=1,3,5$], and (2.7), remains then valid in the neighborhood of $r=0$.

Assuming that on the positive real r axis the function $Q^2(r)$ has two well-separated zeros t_0 and t_1, between which $Q^2(r)$ is positive, and choosing the phase of $Q(r)$ as shown in Fig. 1, we introduce the definitions

$$L=\frac{1}{2}\int_\Gamma q(r)dr, \tag{8.1}$$

where Γ is the closed contour of integration shown in Fig. 1, and

$$K(r_2)=\frac{1}{2}i\int_{\Gamma(r_2)}q(r)dr, \tag{8.2}$$

where $\Gamma(r_2)$ is the nonclosed contour of integration shown in Fig. 1. With the aid of (2.5) we can rewrite (8.2) into the form

$$K(r_2)=\sum_{n=0}^{N}K^{(2n+1)}(r_2), \tag{8.3}$$

where

$$K^{(2n+1)}(r_2)=\frac{1}{2}i\int_{\Gamma(r_2)}Y_{2n}Q(r)dr. \tag{8.4}$$

For $N=0$ the definitions (8.1) and (8.2) go over into (3.9a) and (3.9b), respectively.

The results in the previous sections of the present paper can now directly be generalized to apply to phase-integral approximations of arbitrary order. To this purpose it is only necessary to replace the definitions (3.9a) and (3.9b) by the more general definitions (8.1) and (8.2), respectively. The results (5.9) and (6.7) remain then valid, while in (5.13) one has to replace the integral over $Q^{-1}(r)$ from t_1 to t_2 by half of the integral of $q^{-1}(r)$ over the contour Γ; see Eq. (9) in Ref. 80. We note that the order of the phase-integral approximation used enters into (5.9) only via the value of $K(a)$, obtained from (8.2) with (2.5)–(2.7), but does not appear at all in (6.7) unless the eigenvalues are calculated by means of the phase-integral method.

IX. APPLICATION TO A HYDROGENIC ATOM

For a hydrogenic atom with the charge number Z the potential $V(r)$ in (3.2) is the attractive Coulomb potential

$$V(r)=-Ze^2/r, \quad \text{cgs units}, \tag{9.1}$$

where e is the electron charge. Choosing $Q^2(r)$ according to (2.8b'), we obtain from (3.2) and (9.1)

$$Q^2(r)=R(r)-\frac{1}{4r^2}=\frac{2m}{\hbar^2}[E-V(r)]-\frac{(l+\frac{1}{2})^2}{r^2}. \tag{9.2}$$

When $Q^2(r)$ is chosen according to (9.2), the quantization condition

$$L=(s+\tfrac{1}{2})\pi, \tag{9.3}$$

where L is defined by (8.1), yields the energy levels of the uncompressed hydrogenic atom exactly in the first-order approximation (according to pp. 117–119 in Ref. 65), and since the higher-order contributions to L vanish, the exactness remains in all orders of approximation. Inserting $Q(r)$, obtained from (9.2) and with the phase shown in Fig. 1, into (8.1), and introducing instead of the electron charge e the Bohr radius a_0 defined by

$$a_0=\hbar^2/(me^2), \quad \text{cgs units}, \tag{9.4}$$

we obtain

$$L=\left[\left(\frac{Z^2\hbar^2/(ma_0^2)}{-2E}\right)^{1/2}-\left(l+\frac{1}{2}\right)\right]\pi. \tag{9.5}$$

Inserting (9.5) into (8.3), we find that the energy levels of the uncompressed hydrogenic atom are given by the well-known exact formula

$$E_s^{\infty}=-[Z^2\hbar^2/(ma_0^2)]/2n^2, \tag{9.6}$$

where

$$n=s+l+1 \tag{9.7}$$

is the principal quantum number for the uncompressed hydrogenic atom. We now introduce the effective principal quantum number n_a for the compressed hydrogenic atom by writing in analogy to (9.6)

$$E_s^a=-[Z^2\hbar^2/(ma_0^2)]/2n_a^2. \tag{9.8}$$

As a tends to infinity, n_a must obviously tend to n.

From (9.6)–(9.8) we obtain the exact formula

$$\frac{E_s^a-E_s^{\infty}}{dE_s^{\infty}/ds}=\frac{n(n_a+n)(n_a-n)}{2n_a^2}. \tag{9.9}$$

Noting that n_a is very close to n (since a is assumed to be sufficiently large), we obtain from (5.9) and (9.9) the approximate formula

$$n_a-n=(1/2\pi)(\exp[-2K(a)])_{E=E_s^{\infty}}. \tag{9.10}$$

We shall now evaluate the quantity $K(a)$ for $E=E_s^{\infty}$ up to the third-order approximation. To that purpose it is convenient to introduce as unit of length a_0/Z, which is "the radius of the first Bohr orbit" for the hydrogenic atom with the charge number Z. Therefore we define

$$\tilde{r}=Zr/a_0, \tag{9.11}$$

and put $E=E_s^{\infty}$ in (9.2). From (9.1), (9.2), (9.4), (9.6), and (9.11) we obtain

$$Q(r)dr=\left(-\frac{1}{n^2}+\frac{2}{\tilde{r}}-\frac{(l+\frac{1}{2})^2}{\tilde{r}^2}\right)^{1/2}d\tilde{r}, \quad E=E_s^{\infty}. \tag{9.12}$$

It can easily be shown that the functions Y_{2n} in (2.6a)–(2.6c) can be expressed in terms of the variable $\tilde{r}$ and the quantum numbers n and l. Hence $K(a)$, given by (8.3) and (8.4), can be expressed in terms of the quantum numbers n, l and the parameter

$$\tilde{a}=Za/a_0. \tag{9.13}$$

With the aid of (2.6a), (2.6b), (2.7'), (9.11), (9.12), and (9.13), and with due regard to the contour of integration $\Gamma(r_2)$ shown in Fig. 1, we obtain from (8.4) with $r_2=a>t_1$, after the resulting integrals have been evaluated in the first and third order,

$$\begin{aligned}\exp[-2K^{(1)}(a)]&=\left(\frac{\tilde{a}-n^2+na|Q(a)|}{\tilde{a}-n^2-na|Q(a)|}\right)^n\\&\times\left(\frac{\tilde{a}-(l+\frac{1}{2})^2-(l+\frac{1}{2})a|Q(a)|}{\tilde{a}-(l+\frac{1}{2})^2+(l+\frac{1}{2})a|Q(a)|}\right)^{l+1/2}\\&\times\exp[-2a|Q(a)|], \quad E=E_s^{\infty},\end{aligned} \tag{9.14a}$$

$$\begin{aligned}2K^{(3)}(a)&=\frac{1}{12[n^2-(l+\frac{1}{2})^2][a|Q(a)|]^3}\\&\times(-\tilde{a}^3/n^2+6\tilde{a}^2-3(l+\tfrac{1}{2})^2\tilde{a}^2/n^2\\&-3n^2\tilde{a}-n^2(l+\tfrac{1}{2})^2+2(l+\tfrac{1}{2})^4), \quad E=E_s^{\infty},\end{aligned} \tag{9.14b}$$

where

$$a|Q(a)|=(\tilde{a}^2/n^2-2\tilde{a}+(l+\tfrac{1}{2})^2)^{1/2}, \quad E=E_s^{\infty}. \tag{9.15}$$

In Fig. 3 the accuracy of (9.10), with (8.3) for $r_2=a$ and $N=0$ and 1, (9.14a), (9.14b), and (9.15), is illustrated for the states $1s$ ($n=1$, $l=0$), $2s$ ($n=2$, $l=0$), and $2p$ ($n=2$, $l=1$). The exact values of n_a were obtained from

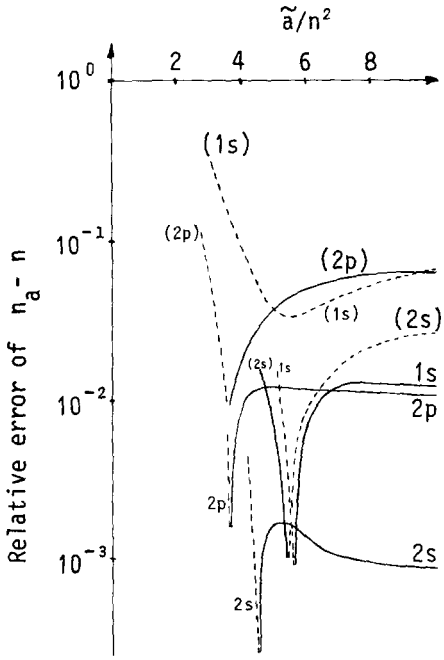

FIG. 3. The relative error of $n_a - n$, i.e.,

$$[(n_a - n)_{\text{approx}} - (n_a - n)_{\text{exact}}]/(n_a - n)_{\text{exact}} = [(n_a)_{\text{approx}} - (n_a)_{\text{exact}}]/(n_a - n)_{\text{exact}},$$

is plotted against $\tilde{a}/n^2 = Za/(a_0 n^2)$ for the states $1s$ ($n = 1$, $l = 0$), $2s$ ($n = 2$, $l = 0$), and $2p$ ($n = 2$, $l = 1$). The figure is based on the choice (9.2) of $Q^2(r)$. As the radius a tends to infinity, n_a tends to n, which is the principal quantum number for the uncompressed hydrogenic atom. Full-drawn lines correspond to positive errors and broken lines to negative errors. It should be mentioned that each cusp in the figure actually corresponds to an error equal to zero, although for practical reasons this is not seen in the figure. The curves with the notations $(1s)$, $(2s)$, and $(2p)$ give results of the first-order phase-integral approximation, and the curves with the notations $1s$, $2s$, and $2p$ give results of the third-order phase-integral approximation. Characterizing the position of the right-hand turning point by the parameter $\tilde{t}_1 = Zt_1/a_0$, we have

$$\frac{\tilde{t}_1}{n^2} = \begin{cases} 2.12, & \text{for } 1s, \\ 2.03, & \text{for } 2s, \\ 2.25, & \text{for } 2p. \end{cases}$$

(9.8) with the use of numerically calculated values of E_s^a. From Fig. 3 it is seen that we obtain in general a considerable improvement of the accuracy by taking the third-order correction into account. Furthermore, as the radius a decreases, the approximations finally deteriorate and in fact break down when a comes too close to the turning point t_1.

For fixed l one finds from (9.6), (9.7), and (9.8) that the ratio of the increase of the energy level E_s^∞ due to the compression and the energy difference between the uncompressed energy levels with the quantum numbers s and $s+1$ is approximately

$$\frac{E_s^a - E_s^\infty}{E_{s+1}^\infty - E_s^\infty} = \frac{2(n+1)^2}{n(2n+1)}(n_a - n). \tag{9.16}$$

The factor in front of $n_a - n$ in the right-hand member of (9.16) is a monotonically decreasing function of n which is equal to $\frac{8}{3}$ for $n = 1$, equal to $\frac{9}{5}$ for $n = 2$, and equal to 1 for $n = \infty$. The ratio in the left-hand member of (9.16) is therefore roughly equal to $n_a - n$.

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An investigation of (nonadditive) scattering invariants in classical mechanics and quantum theory by differential topological methods

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The structure of invariants of the scattering transformation in (relativistic and nonrelativistic) classical mechanics and quantum theory is investigated and a constructive approach to finding and classifying them by exploiting and developing certain differential topological methods is provided. While, in the form of various by-products, results about the perhaps better known so-called additive scattering invariants are (re)derived, the primary concern here is with the less well-known nonadditive (i.e., several particle) conserved quantities.

I. INTRODUCTION

The computation of the so-called integrals of motion in the classical mechanics of mass points is both a very old and (at least in general) difficult problem. It is well known that the number of independent integrals of motion for a closed mechanical system with n degrees of freedom is $2n-1$ (cf. Ref. 1) with an additive time constant being eliminated. For a Hamiltonian system a function $f \in C^1$ depending on the positions $\{q_k\}$ and momenta $\{p_k\}$ is an invariant along every path of motion iff

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \{H,f\} = 0 \tag{1.1}$$

with H the Hamiltonian and

$$\{H,f\} = \sum_k \frac{\partial H}{\partial_{p_k}} \cdot \frac{\partial f}{\partial_{q_k}} - \frac{\partial F}{\partial_{q_k}} \cdot \frac{\partial f}{\partial_{p_k}} . \tag{1.2}$$

Since we are in the following primarily dealing with systems in the usual Cartesian space we alter the notation slightly denoting positions by x_k, momenta by $p_k, x_k, p_k \in \mathbb{R}^3$ with $p_k = m_k \cdot \dot{x}_k$. This implies that we will not rely on the heavy abstract machinery being developed, for example, in the book of Abraham[2] and more recent ones devoted to the study of the properties of general dynamical systems. Instead we would like to emphasize a certain conceptual relationship between the things we will discuss and related problems in quantum scattering theory and quantum field theory.

In this more general context one is interested in symmetries of the scattering matrix S and how classical mechanics fits in a very natural way into this general scheme. One can then ask a slightly more general question. Instead of looking for physical quantities conserved along the whole path of the system (with the necessary modifications of this picture in quantum theory) one can direct one's attention to symmetries or invariants of the S matrix, that is, observables asymptotically invariant under time evolution and approaching the same limits along each trajectory for time $t \to \pm\infty$. Investigations of the long time phenomena within classical mechanics by means of notions and strategies developed originally in quantum scattering theory can be found, e.g., in Refs. 3–6. We want, however, to remark that our approach is so general that it can be easily extended to more abstract dynamical systems.

We assume an interacting and a free time evolution to be given defining flows ϕ_t, ϕ_t^0:

$$\phi_t : (x(0),p(0)) \to (x(t),p(t)), \quad x,p \in \mathbb{R}^{3n}. \tag{1.3}$$

We define the so-called "Möller transformations" $\Omega_\pm$,

$$\Omega_\pm := \lim_{t \to \mp\infty} \phi_{-t} \cdot \phi_t^0, \tag{1.4}$$

assumed to exist on certain sets $D_\pm \subset \mathbb{R}^{6n}$, which we expect to be the set of initial conditions of all the free orbits up to certain sets of Lebesque measure zero.

As in quantum theory the situation can be relatively easily controlled in the two-body case or for single particle scattering in an external potential. For the n-particle case one has in principle to admit for the possibility of various channels, i.e., clusters of "bound" particles moving freely in the limits $t \to \pm\infty$. While in our approach the number of particles (resp. clusters) moving to infinity for $t \to +\infty$ is allowed to differ from the number of "ingoing" ones, we prefer to not overburden the formalism with these details and assume that all particles are unbound as $t \to \pm\infty$. (The necessary machinery to deal with bound clusters of particles, e.g., channel Hamiltonians, cluster decompositions and all that, can be found in Ref. 5 and is basically the same as in quantum scattering.) Thus we have to exclude the initial conditions for the free comparison dynamics (note that these are the phase space coordinates at $t=0$), where some of the relative momenta are zero. With this proviso we assume the admissible initial conditions to be $\mathbb{R}^{6n}$ up to sets of measure zero (as to more details and the various notions of asymptotic completeness in the single particle case we refer the reader, for example, to Chap. XI.2 of Ref. 4).

The S transformation defined by

$$S := (\Omega_-)^{(-1)} \cdot \Omega_+ \tag{1.5}$$

then maps free asymptotes at $t = -\infty$ onto the corresponding ones at $t = +\infty$. The free orbits

$$x_i^0(t) = x_i^o + p_i/m_i \cdot t \tag{1.6}$$

are mapped by the Möller transformations onto the corresponding time zero coordinates of the interacting system

$$\Omega_\pm : \{x_i^0, p_i\} \to \{x_i(0), p_i(0)\} \tag{1.7}$$

called

$$\{x_i^{\text{in}}, p_i^{\text{in}}\} \quad (\text{resp. } \{x_i^{\text{out}}, p_i^{\text{out}}\})$$

and the S transformation

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$$S:\ \{x_1p_1,\ldots,x_np_n\}\to\{x'_1p'_1,\ldots,x'_np'_n\} \tag{1.8}$$

(where for notational simplicity we supress the superscript 0).

Remark: We discuss only the case of short-range potentials. For long-range potentials the asymptotes have to be slightly modified (cf. Ref. 4 Chap. XI.9).

Definition 1: Invariants of the S transformation are functions F such that (s.t.)

$$\text{(i)}\ F(x_1p_1,\ldots,x_np_n)=F(x'_1p'_1,\ldots,x'_np'_n), \tag{1.9}$$

where the coordinates on the lhs and rhs are the pairs occurring in a scattering event with the additional property of being constant along free paths; i.e.,

$$\text{(ii)}\ F(x_1^o(t)p_1,\ldots,x_n^0(t)p_n)=F(x_1^o(t')p_1,\ldots,x_n^o(t')p_n) \tag{1.10}$$

(in principle we could admit an F', n' different from F,n on the rhs).

Perhaps a little bit surprisingly, quantum and quantum field theory (without spin) can be treated along the same lines. We assume a self-adjoint operator Q to be given on the n-particle states of the free time evolution. If Q is the generator of a symmetry it usually can be represented on the free states by a certain sum of terms consisting of products of functions $f_i(x_1,\ldots,x_n)$ and expressions in $\partial_{x_1},\ldots,\partial_{x_n}$, i.e.,

$$Q\hat{=}\sum_i f_i(x_1,\ldots,x_n)\cdot P_i(\partial_1,\ldots,\partial_n). \tag{1.11}$$

If Q commutes with S we have

$$(\varphi,S\cdot Q\psi)=(Q\varphi,S\psi), \tag{1.12}$$

which implies for the scattering amplitude $S(x_1,\ldots,x_n;x'_1,\ldots,x'_n)$ (actually a certain distribution)

$$\Big\{\sum_i f_i(x_1,\ldots,x_n),P_i(\partial_{x_1},\ldots,\partial_{x_n})-\sum_i f_i(x'_1,\ldots,x'_n)\times P_i(\partial_{x_1},\ldots,\partial_{x_n})\Big\}\cdot S(x_1,\ldots,x_n;x'_1,\ldots,x'_n)\equiv 0 \tag{1.13}$$

and a corresponding expression in momentum space which is particularly useful for symmetries commuting with the space translations. In this special case we get

$$\{P(p_1,\ldots,p_n)-P(p'_1,\ldots,p'_n)\}\cdot S(p;p')\equiv 0. \tag{1.14}$$

If there is scattering *at all*, i.e., a certain *open* set on the scattering manifold where $S(p;p')$ is nontrivial, the expression in the curly brackets has to vanish identically on this set, a situation completely analogous to the classical one.

The investigation of symmetries of the S matrix focussed mainly on so-called additive or summation invariants, notions being explained later, leading to perhaps a little bit puzzling: "no go theorems," usually of the tenor that there exist no more additive invariants (apart from inner symmetries) than the *a priori* ones already known. In quantum field theory many papers were initiated by a result of this type by Coleman and Mandula[7] (cf. also Refs. 8 and 9 and previously Ref. 10). As to classical mechanics the history is of course much longer and we want to give only a few references. Results of this type have been of particular interest in kinetic gas theory (cf., e.g., Refs. 11 and 12), and belonged in a certain sense to the general folklore in this field. The situation was then more carefully studied by Grad,[13] who remarks that the situation is far from obvious, and quite recently by Amigo and Reeh,[14] where further references (e.g., for relativistic dynamics) can be found. In this context, with particular emphasis on relativistic particle scattering, one should also mention the original approach to the whole subject matter given in Ref. 15.

While our investigation will, in the form of various by-products, also yield results about additive conservation laws its main impetus is, however, directed towards the much less well known but probably more important regime of *nonadditive* scattering invariants. Since, for example, all $2n-1$ initial conditions are by definition invariants of motion in classical mechanics [when being expressed as functions of the actual $x_i(t),p_i(t)$], while, on the other side, the number of additive ones usually does not exceed 10, it is quite apparent that the former set is not empty. It is, however, both difficult to extract them from the concretely given model theories and, *a fortiori*, to characterize them by means of more general principles. Some steps in this direction can, e.g., be found in the classical book of Whittaker,[16] the perhaps most notable result in this direction being the theorem of Bruns, viz., there are no other *algebraic* invariants of motion in celestial mechanics of three bodies than the already known ones. [Note that (i) in the case of two bodies there does exist an additional one, namely the so-called Runge–Lenz vector; and (ii) the emphasis lies on "algebraic," which implies that while additional invariants do exist they are necessarily of a complicated (transcendental) type and therefore difficult to find.]

In quantum field theory the situation is (understandably) less transparent, in particular concerning existence and properties of objects corresponding to the nonadditive scattering invariants of classical mechanics. A possibly analogous role might be played by multilocal conserved quantities (called charges in this field). These objects have been found in some lower-dimensional models and in a recent paper Buchholz, Lopuszanski, and Rabsztyn[17] (see also Refs. 18 and 19) try to develop an approach allowing us to systematically study them in the physical relevant dimension 4. It may be promising to try to relate these ideas with our strategy, which is different, in the future.

Our approach, in contrast to most of the papers mentioned above, carries a distinctive differential topological flavor. Its advantages are (in our view) that it allows us to study these and more general questions on a considerably broader scale and in a concise and unified manner, i.e., the same methods work in classical mechanics, quantum theory, and quantum field theory (QFT). Even in the much better understood situation of additive invariants it sheds some new light upon some of the perhaps more hidden aspects of the problems under discussion.

To mention a few: (i) it does not need the existence of a regime where particles scatter only elastically; (ii) the somewhat hidden but (in fact) for many conclusions crucial and nontrivial assumption of the existence of certain suitable open sets on the scattering manifold being coverable by real scattering events is brought to light, leading, on the other side, to a fine structure within the class of scattering invar-

iants; and (iii) it might perhaps be easier to extend our approach to more complicated invariants in QFT having, e.g., a tensor (resp. spinor) character of a higher degree. This represents still a major obstacle in extending the classical Coleman–Mandula result to higher charges. Also (iv) since neither the particle number nor the shape of the function F has to be the same for in- (resp. out-) states, the approach can be easily extended to objects (charges) which do not commute with the S matrix! This topic and the extension to general charges in quantum field theory will, however, be given elsewhere.

The paper is organized as follows: In Sec. II we transform the problem into a purely mathematical one thus displaying what sort of treatment is actually the appropriate one, what belongs to the physical input, and what is the mathematical machinery. We then discuss in Sec. III in a first step invariants depending only on the momenta of the scattering partners and derive various structure theorems for them as, e.g., every nonadditive invariant depending only on the momenta is a function of overall energy and momentum (in most cases even a polynomial). In Sec. IV we carefully analyze the physical side of the problem, in particular, the structure of the set of in- and out-states being connectable by the scattering transformation. Section V deals with the structure of invariants depending on the momenta, positions, and the time. The results are, however, less complete and cover only the field of classical mechanics (in order not to overburden the paper). It is exactly at this point where future work has to set in. In the last section, which has more the character of an appendix, we discuss an explicit counterexample against the usual physical intuition, i.e., the potential $V(r) \sim r^{-2}$.

II. THE MATHEMATICAL SIDE OF THE PROBLEM

We begin with the subclass of invariants depending only on the momenta of the asymptotic particles. Furthermore, we restrict ourselves, for the time being, to functions from $C^1(\mathbb{R}^{3n})$. It is not clear to us whether one really loses something by not considering more nasty functions in this special context. In any case, by smearing with appropriate test functions, one can usually extend the results to more general invariants (if there are any) (see, e.g., Ref. 14).

This question is, however, not purely academic. Take, e.g., one of the Cauchy equations over $\mathbb{R}$:

$$f(x+y) = f(x) + f(y). \tag{2.1}$$

Assuming f to be in C^1 the construction of a solution is very easy. We have

$$f'(x+y) = f'(x) = f'(y), \quad f(0) = f(0) + f(0), \tag{2.2}$$

from which

$$f(0) = 0, \quad f'(x) = \text{const}, \quad \text{i.e., } f(x) = a \cdot x, \tag{2.3}$$

follows. In a next step one usually tries to prove that possible solutions lying in a more general class are automatically differentiable. There is, for example, the result that a solution being locally Lebesgue integrable is already $\in C^1$. On the other hand there do exist *nonmeasurable* solutions(!) (cf. the history of this equation given in Ref. 20, Chap. 14.2 or in Ref. 15).

Let p_i, $\epsilon_i(p_i)$, $i = 1,\ldots,n$ be the momenta and energies of the asymptotic particles. Energy-momentum conservation then forces the ingoing and outgoing momenta to lie in a certain subset of $\mathbb{R}^{3n} \times \mathbb{R}^{3n}$, i.e., we present the following definition.

Definition 2: The scattering manifold $M \subset \mathbb{R}^{3n} \times \mathbb{R}^{3n}$ in momentum space is defined by the four constraints

$$\begin{aligned} &\sum_{i=1}^{n} p_i - \sum_{i=1}^{n} p_i' = 0, \\ &\sum_{i=1}^{n} \epsilon_i(p_i) - \sum_{i=1}^{n} \epsilon_i(p_i') = 0, \end{aligned} \tag{2.4}$$

with $p_i \in \mathbb{R}^3$, $\epsilon_i(p_i) \in C^1$, away from possibly a certain set of discrete points. The corresponding Jacobi matrix is assumed to have rank 4, i.e., the constraints are assumed to be *independent*. In more modern language,

$$\begin{aligned} &f\colon \mathbb{R}^{6n} \to \mathbb{R}^4, \\ &(p_1,\ldots,p_n;p_1',\ldots,p_n') \\ &\quad \to \left(\sum p_i - \sum p_i', \sum \epsilon_i(p_i) - \sum (p_i') \right) \end{aligned} \tag{2.5}$$

does not have $0 \in \mathbb{R}^4$ as a *critical value*. (As to this notion cf., e.g., Ref. 20.)

Remarks: (i) In applications $\epsilon(p)$ is usually $\in C^\infty$ away from possibly $p = 0$, e.g., $\epsilon(p) = c \cdot p^2$, $\sqrt{p^2 + m^2}$, etc., $\epsilon(p) = c \cdot |p|$ may serve as an example for an $\epsilon(p)$ not $\in C^1$ in $p = 0$.

(ii) As to the assumed independence of the above four constraints, one should say that this is the usual state of affairs (e.g., for particles with nonzero mass). There exist, however, even in physics, illuminating counterexamples. In principle two situations can occur in general:

(α) rank $f < 4$ at a point but is, nevertheless, locally constant (the rank is locally lower continuous anyway);

(β) rank $f < 4$ but is locally nonconstant, i.e., it increases (discontinuously) in every neighborhood of that point. (2.6)

In case (α) the situation is still relatively smooth. The codimension of M is simply < 4. However, (β) is much more singular. The codimension of M (which, in general, may even no longer be a true submanifold of $\mathbb{R}^{m \cdot n}$) may increase abruptly to values > 4 at some points s.t. the set M may turn out to be much smaller than expected. This can also happen in physics: Take, e.g., disintegration of a zero mass particle into two others:

$$p_1 = p_1' + p_2', \quad |p_1| = |p_1'| + |p_2'| \text{ implying } p_1' \| p_2'. \tag{2.7}$$

That is, we get actually five constraints for the momenta p_1, p_1', p_2' from the four equations (2.4). The codimension of M is now 5 instead of 4 (one of the typical phase space constraints in photon scattering). Stated differently, the map (2.5) has 0 as a critical value and (β) applies. We assume this phenomenon to be absent in the following.

As was already remarked in Ref. 14 the whole manifold M is not usually accessible to concrete scattering experiments. On the other hand this is an important point since

almost all the classical proofs relied *heavily* on this assumption. Solutions of the equations of motion are usually given uniquely by their initial conditions. But one has a certain freedom in varying, e.g., the impact parameter while keeping the ingoing momenta fixed, thereby varying the outgoing momenta. These physical aspects of the problem will be discussed in detail in Sec. IV. So let us for the moment simply assume that, while the whole M usually cannot be covered by scattering events for a given *fixed* interaction between the particles, there exists at least an *open* set $U \subset M$ corresponding to a concrete scattering situation. Thus we have the following definition.

Definition 3: A function $F(p_1,...,p_n) \in C^1(\mathbf{R}^{3n})$ is called an *invariant* of the scattering transformation of the *first kind* iff for a certain *open* subset $U \subset M$ we have the relation

$$F(p) - F(p') \equiv 0 \quad \text{for all } (p,p') \in U \tag{2.8}$$

[with p, p' standing for the n-tuples $(p_1,...,p_n)$, $p_1',...,p_n'$)]. This implies $\dim(U) = \dim(M) = (6n-4)$. The general mathematical situation is, however, more involved. With $P' := \Sigma p_i^{(\prime)}$, $E^{(\prime)} := \Sigma \epsilon_i(p_i^{(\prime)})$, M was defined as the intersection of the four hypersurfaces given by energy-momentum conservation. If one looks for further conserved quantities, say F, what has to be usually expected is the relation $F(p) = F(p')$ to hold on M only on a submanifold of dimension $< 6n - 4 - 1$, the intersection of the hypersurface given by the additional conservation law with M. That is, we have the following.

Definition 4: The function F, given in Definition 3, is called an invariant of the *second kind* iff relation $F(p) \equiv F(p')$ holds only a subset $U' \subset U \subset M$ of dimension $d < 6 \cdot n - 5$.

Geometric observation: If the situation is the one described in Definition 3 M is at least locally *contained* in the hypersurface defined by F. Definition 4 describes the phenomenon that this hypersurface hits M *transversally*, thus reducing the dimension by at least 1 (as to more details concerning these notions cf. Ref. 21.

Physical observation: Let $M_p \subset M$ denote the (physical) submanifold which can be covered by real scattering experiments. Under the assumption of Definition 3 $\dim(M)_p = \dim(M)$. Since the momenta of the ingoing particles can always be freely chosen we have $\dim(M)_p \geqslant 3n$ in general. We show in Sec. IV that in the pure momentum case $\dim(M)_p = \dim(M)$. In the case of more general invariants this will, however, never hold! In that case, i.e., $\dim(M)_p < \dim(M)$, Definition 4 becomes relevant.

Whether there are such invariants of the second kind requires a careful analysis of the physical scattering situation and this will be given in Sec. IV. In any case there exists a very useful structure theorem that allows us to discriminate between these two possibilities. For its proof we need the following simple lemma.

Lemma 1: Let $f \in C^1$ be a function of an open neighborhood $\tilde{U}$ of $0 \in \mathbf{R}^n \times \mathbf{R}^k$, the coordinates denoted by $(x_1,...,x_n; y_1,...,y_k)$. The following is assumed to hold:

$$f | \tilde{U} \cap (\mathbf{R}^n \times \{0\}) \equiv 0.$$

Then f can be written in a full open neighborhood $\tilde{U}' \subset \tilde{U}$ of $0 \in \mathbf{R}^n \times \mathbf{R}^k$ in the form

$$f = \sum_{i=1}^{k} y_i \cdot f_i, \quad f_i \in C \text{ with respect to } y. \tag{2.9}$$

Proof:

$$f(x,y) = f(x,0) + \int_0^1 \frac{d}{dt} f(x, t\cdot y)\, dt,$$

$$= \sum_{i=1}^{k} y_i \cdot \int_0^1 \partial_{ty_i} f(x, t\cdot y)\, dt. \tag{2.10}$$

Let now U be open on M s.t. $F(p) = F(p')$ holds on U. Since M is given by the relations

$$P - P' \equiv 0, \quad E - E' \equiv 0,$$

with the corresponding Jacobi matrix having rank 4 on U, we can choose *local coordinates* in an open neighborhood $\tilde{U} \supset U$, $\tilde{U}$ open in $\mathbf{R}^{3n} \times \mathbf{R}^{3n}$! We obtain

$$(\tilde{x}_1,...,\tilde{x}_{6n-4}; \tilde{y}_1,...,\tilde{y}_4)$$

s.t. (2.11)

$$\tilde{y}_1 := P_1 - P_1',...,$$

$$\tilde{y}_3 := P_3 - P_3', \quad \tilde{y}_4 := E(p) - E(p'),$$

that is, with $\tilde{y}_i$ a basis of local coordinates being normal to M. With the help of Lemma 1 we can now prove the following proposition.

Proposition 1: Let U be open on M s.t. $F(p) = F(p')$ on U holds with F given in Definition 3. We have then in a neighborhood $\tilde{U} \supset U$, $\tilde{U}$ open in $\mathbf{R}^{3n} \times \mathbf{R}^{3n}$, the representation

$$F(p) - F(p') = \sum_{i=1}^{3} (P_i - P_i') \cdot G_i(p,p') + (E(p) - E(p')) \cdot G_4(p,p') \tag{2.12}$$

with $G_i, G_4 \in C(\mathbf{R}^{3n} \times \mathbf{R}^{3n})$, $P, P', E(p), E(p')$ the overall momentum and energy of the ingoing and outgoing particles, and P_i, e.g., denoting the ith component of P.

Proof: $\tilde{U}$ is diffeomorphic to a neighborhood of $0 \in \mathbf{R}^{6n-4} \times \mathbf{R}^4$ with $\tilde{y}_i = P_i - P_i'$, $\tilde{y}_4 := E - E'$ locally spanning $\mathbf{R}^4$. Here $F(p) - F(p')$ corresponds to a certain function $\tilde{F}(\tilde{x},\tilde{y})$ defined around $0 \in \mathbf{R}^{6n-4} \times \mathbf{R}^4$ with $\tilde{F} | (\tilde{U} \subset \mathbf{R}^{6n-4} \times \{0\}) \equiv 0$ (since F is supposed to be conserved on M). By Lemma 1 we see that F has a representation

$$\tilde{F}(\tilde{x},\tilde{y}) = \sum \tilde{y}_i \cdot G(\tilde{x},\tilde{y}) + \tilde{y}_4 \cdot G_4(\tilde{x},\tilde{y}). \tag{2.13}$$

Reinserting the original coordinates $\{p_1,...,p_n; p_1',...,p_n'\}$ proves the statement.

If we have the identity $F(p) - F(p')$ only on a submanifold of smaller dimension than M itself the above local coordinate system would be not exhaustive. The local coordinate which is missing may just belong to a hidden independent conservation law or to F itself. In any case, $F(p) - F(p')$ *cannot* be represented in the form (2.12) when this happens to be the case.

III. A CONSTRUCTIVE DETERMINATION OF THE FUNCTIONAL FORM OF (NON)ADDITIVE INVARIANTS (PURE MOMENTUM CASE)

This section contains the bulk of the technical aspects of our approach together with a complete classification of gen-

eral invariants depending only on the momenta. Invariants depending also on the positions are treated in Sec. V. A crucial role will be played by our structure theorem (2.12). We will exploit the peculiar form of (2.12), i.e., that the lhs is the difference of two functions depending solely on either p or p'. To that end we will differentiate both sides with respect to p_i, p'_j, $i,j = 1,\ldots,n$, assuming, in order that the G_i's be $\in C^1$, that $F \in C^2$. We then get

$$\begin{aligned} \partial_{p_i} F(p) = \mathbf{G}(p,p') &+ (P_\nu - P'_\nu)\cdot \partial_{p_i} G_\nu(p,p') \\ &+ \partial_{p_i}\epsilon_i(p_i)\cdot G_4(p,p') \\ &+ (E(p) - E(p'))\cdot \partial_{p_i} G_4(p,p'), \end{aligned} \tag{3.1}$$

with $\mathbf{G}$ the vector with components G_ν, $\nu = 1,2,3$, and an analogous result for p'_j.

Choosing (p,p') to lie *a fortiori* on M we have $(P_\nu - P'_\nu) = (E(p) - E(p')) = 0$, that is

$$\begin{aligned} &\partial_{p_i} F(p)\,|\,U = \mathbf{G}(p,p') + \partial_{p_i}\epsilon_i(p_i)\cdot G_4(p,p'), \\ &\partial_{p'_j} F(p')\,|\,U = \mathbf{G}(p,p') + \partial_{p'_j}\epsilon_j(p'_j)\cdot G_4(p,p'). \end{aligned} \tag{3.2}$$

The expressions (3.2) and the corresponding ones in the more complicated situations dealt with in Sec. V will turn out to be of particular use in calculating invariants. What we have in fact achieved by using this simple trick is that the lhs of (3.2) depends either solely on p or p' while on the rhs there are terms, $\mathbf{G}$, G_4, which are independent of the subscript i,j!

We proceed now as follows: In a first step we get

$$\begin{aligned} \mathbf{G}(p,p') &= -\partial_{p_i}\epsilon_i(p_i)\cdot G_4(p,p') + \partial_{p_i} F(p), \\ \mathbf{G}(p,p') &= -\partial_{p'_j}\epsilon_j(p'_j)\cdot G_4(p,p') + \partial_{p'_j} F(p') \end{aligned} \tag{3.3}$$

which holds on $U \subset M$ and for all i,j. This expression can be exploited in various ways. The lhs is completely independent of the index i (resp. j). So, taking the derivative in the first (second) expression with respect to p_i, p_j (p'_l, p'_k), subtracting the corresponding equations from each other and bringing G_4 to the left-hand side we arrive at

$$\begin{aligned} G_4(p,p') &= (\partial^{(\nu)}_{p_i} F(p) - \partial^{(\nu)}_{p_j} F(p)) \\ &\quad \times (\partial^{(\nu)}_{p_i}\epsilon_i(p_i) - \partial^{(\nu)}_{p_j}\epsilon_j(p_j))^{-1}, \\ G_4(p,p') &= (\partial^{(\nu)}_{p'_l} F(p') - \partial^{(\nu)}_{p'_k} F(p')) \\ &\quad \times (\partial^{(\nu)}_{p'_l}\epsilon_l(p') - \partial^{(2)}_{p'_k}\epsilon_k(p'_k))^{-1} \end{aligned} \tag{3.4}$$

(no summation over ν!), which holds on U where the superscript ν denotes the νth component of the gradient. Reinserting this into (3.3) we get a corresponding explicit expression for $\mathbf{G}$. We observe the remarkable fact that both the rhs of (3.4) and after having inserted the lhs of (3.4) into (3.3) the rhs of (3.3) depend either solely on p or p' while $\mathbf{G}(p,p')$, $G_4(p,p')$ are, in principle, functions of both p and p'. This will be exploited in the following way.

While away from the scattering manifold, M, $\mathbf{G}$, G_4 are expected to depend both on p and p', we see that on M, i.e., the subset of pairs (p,p') which can be related via a scattering process, we have

$$\begin{aligned} G_\nu(p,p') &= G_\nu(p) = G_\nu(p'), \\ G_4(p,p') &= G_4(p) = G_4(p'). \end{aligned} \tag{3.5}$$

But this is exactly the condition a scattering invariant has to fulfill! That is, we have the following theorem.

Theorem 1: With $F \in C^2$ being a scattering invariant on an open neighborhood U on M, i.e., $F(p) = F(p')$, $(p,p') \in U$, there exists a neighborhood $\tilde{U} \supset U$, open in $\mathbb{R}^{3n} \times \mathbb{R}^{3n}$, s.t.

$$F(p) - F(p') = G^\nu \cdot (P_\nu - P'_\nu) + G^4 \cdot (E(p) - E(p'))$$

holds on $\tilde{U}, G^\nu, G^4 \in C^1$ with respect to (p,p'). Here G^ν and G^4 have the remarkable property that they are themselves scattering invariants, i.e., we have

$$\left.\begin{aligned} G^\nu(p,p') = G^\nu(p) = G^\nu(p') \\ G^4(p,p') = G^4(p) = G^4(p') \end{aligned}\right\} (p,p') \in \mathbf{M}.$$

Here G^ν and G^4 are explicitly given on M by the expressions (3.3) and (3.4).

Before we proceed to deal with the more complex situation we would like to discuss the special class of so-called *additive* invariants.

Definition 5: An invariant, $F(p)$, of the scattering transformation is called additive iff

$$F(p) = \sum_{i=1}^{n} f_i(p_i). \tag{3.6}$$

In this particular case the relations (3.3) and (3.4) can be readily exploited showing that G^ν and G^4 are on M functions of any of the couples (p_i, p_j) [resp. (p'_l, p'_k)], $i \neq j$, $k \neq l$. This shows that, in fact G^ν and G_4 cannot really depend on *any* of these couples on M, that is, we have

$$G_4 = \text{const}, \quad G^\nu = \text{const} \quad \text{on } M. \tag{3.7}$$

By (3.2) we get

$$\partial^{(\nu)}_{p_i} f_i(p_i) = C_\nu + \partial_{p_i}\epsilon_i(p_i)\cdot C_4 \quad \text{on } M, \tag{3.8}$$

which implies

$$f_i(p_i) = C_\nu \cdot p_i^{(\nu)} + C_4\epsilon_i(p_i) + C_{0,i}, \tag{3.9}$$

with C_ν, C_4 being *independent* of the index $\{i\}$. That is, we have the following theorem.

Theorem 2: For an additive conserved quantity, $F(p) = \Sigma_{i=1}^n f_i(p_i)$, on $U \subset M$ we have the relation (3.9), that is,

$$F(p) = C_\nu \cdot P^{(\nu)} + C_4 \cdot E(p) + C_0, \tag{3.10}$$

i.e., a superposition of momentum, energy, and a constant. We want to come now to the main topic of this investigation, i.e., the structure of nonadditive scattering invariants. This is an extremely difficult subject matter and very little is known. We mention in this context, e.g., the classical book of Whittaker,[16] where, properly speaking, invariants of motion are discussed and Ref. 17 in the case of QFT. The machinery being developed in this chapter will turn out to be sophisticated enough to give an exhaustive answer in the restricted case of invariants depending only on the momenta. Many of the calculational steps can, however, be carried over to invariants depending also on the positions of the particles and the time but this will be a much more ambitious program with partial answers being given in Sec. V.

We have the following theorem.

Theorem 3: (i) Under the same assumptions as in Theorem 1 every scattering invariant depending only on the momenta is a function of overall energy E and momentum P provided that the map $\{p \to \partial_p \epsilon(p)\}$ is a homeomorphism

a.e., i.e.,

$$F(p_1,\ldots,p_n)=F\left(\sum \epsilon_i(p_i),\ \sum p_i\right). \tag{3.11}$$

(ii) Furthermore, if F is an m-particle observable with $f\in C^m$ and $m<n$, i.e.,

$$F(p_1,\ldots,p_n)=\sum_{\{i_1,\ldots,i_m\}} f_{\{\cdots\}}(p_{i_1},\ldots,p_{i_m}),$$

then f is at most a polynomial of mth order in the variables p_i,ϵ_i of the form (3.25).

Remarks: (i) Note that the result holds also in quantum field theory for translationally covariant charges.

(ii) The crucial part is (i), i.e., (3.11). The idea that also (ii) should hold (which is obvious for polynomials) was inspired by an observation made in Ref. 15 in the special case of relativistic three-particle scattering and a two-particle scattering invariant. The assumption $m<n$ is crucial for the proof. This is, however, not a series drawback since in many cases one can simply add more particles in order to make n bigger than m for fixed given $f(p_1,\ldots,p_m)$.

Proof: (i) As before we choose a special local coordinate system in R^{3n}, the first four local coordinates being P and E, the remaining $3n-4$ being denoted by $\zeta:=\{\zeta_1,\ldots,\zeta_{3n-4}\}$ and consider F as a function of E,P,ζ. Employing Eq. (3.2) we get $(\partial_\zeta F:=(\partial_{\zeta_1}F,\ldots,\partial_{\zeta_{3n-4}}F),\ \partial_{p_i}\zeta:=(\partial_{p_i}\zeta_1,\ldots))$

$$\partial_P F+\partial_E F\cdot\partial_{p_i}\epsilon(p_i)+\partial_\zeta F\cdot\partial_{p_i}\zeta$$
$$=\mathbf{G}+G_4\cdot\partial_{p_i}\epsilon(p_i)\quad\text{for all } i, \tag{3.12}$$

$$\partial_E F\cdot(\partial_{p_i}\epsilon(p_i)-\partial_{p_j}\epsilon(p_j))+\partial_\zeta F\cdot(\partial_{p_i}\zeta-\partial_{p_j}\zeta)$$
$$=G_4\cdot(\partial_{p_i}\epsilon(p_i)-\partial_{p_j}\epsilon(p_j)), \tag{3.13}$$

implying

$$G_4=\partial_E F+\partial_\zeta F\cdot\{(\partial_{p_i^\nu}\zeta-\partial_{p_j^\nu}\zeta)$$
$$\times(\partial_{p_i^\nu}\epsilon_i(p_i)-\partial_{p_j^\nu}\epsilon_j(p_j))^{-1}\} \tag{3.14}$$

or

$$(G_4-\partial_E F)=\partial_\zeta F\cdot\{\cdots\}\quad\text{for all } i\neq j,\ \nu=1,2,3.$$

If we can show that $\partial_{\zeta_\alpha}F=0$ for all α, we have shown that F does depend only on E and P. For technical reasons we will now choose an especially well-adapted local coordinate system, i.e., in addition to P, E, we can take, e.g.,

$$\zeta_1:=p_2^2,\ldots,\zeta_{3n-4}:=p_n^3. \tag{3.15}$$

The map: $(p_1,\ldots,p_n)\to(P,p_2,\ldots,p_n)$ is a diffeomorphism. The same holds for the map: $(P,p_2,\ldots,p_n)\to(E,P,p_2^2,\ldots,p_n^3)$ [with E understood as the function $\epsilon_1(P-p_2-\ldots-p_n)+\epsilon_2(p_2)+\ldots+\epsilon_n(p_n)$] around points where $\partial\epsilon_1/\partial p_2^1\neq 0$. Since there is nothing special about the coordinate p_2^1 it is enough to have $\partial\epsilon_i/\partial p_i\neq 0$ at some point and for some index i in order that the following holds true in a neighborhood of that point.

In this new coordinate system the curly bracket of (3.14) becomes particularly simple. Making the special choice $p_i^\nu=p_1^1,\ p_j^\nu=p_2^1$ we have $(\partial_{p_1^1}\zeta-\partial_{p_2^1}\zeta)\equiv 0$ and hence

$$G_4=\partial_E F\quad\text{on } U\subset M! \tag{3.16}$$

Inserting this into (3.12) we get

$$\partial_P F+\partial_\zeta F\cdot\partial_{p_i}\zeta=\mathbf{G}\quad\text{for all } i. \tag{3.17}$$

With $i=1$ we get $\partial_{p_1}\zeta=0$ (since ζ depends by definition only on $p_2^2,\ldots$). That is, we have by the same token

$$\mathbf{G}=\partial_P F\quad\text{which implies}\quad\partial_\zeta F\cdot\partial_{p_i}\zeta=0\ \text{on } U\ \text{for } \textit{all } i! \tag{3.18}$$

From this we can infer that $\partial_{p_i^\nu}F=0$ for $3(i-1)+\nu\geq 5$, that is, F does not depend on ζ at all, in other words,

$$F(p_1,\ldots,p_n)=F(E,P). \tag{3.19}$$

The proof of the second part of the theorem is almost entirely a consequence of the structure formula (3.19), i.e., given (3.19) the statement is more or less independent of the specific context under discussion. Let $F(p_1,\ldots,p_n)$ have the functional form

$$F(p_1,\ldots,p_n)=F(E,P)=\sum_{\{i_1,\ldots,i_m\}} f_{\{\cdots\}}(p_{i_1},\ldots,p_{i_m}),\quad m<n, \tag{3.20}$$

with $F\in C^m(R^{3m})$. From (3.20) we infer that

$$\partial_{p_{i_1}^{\alpha_1}}\cdots\partial_{p_{i_m}^{\alpha_m}}F(E,P)=\partial_{p_{i_1}^{\alpha_1}}\cdots\partial_{p_{i_m}^{\alpha_m}}f_{\{\cdots\}}(p_{i_1},\ldots,p_{i_m}) \tag{3.21}$$

holds for an arbitrary but fixed index set $\{i_1,a_1;\ldots;i_m,a_m\}$.

The following calculation can be done without difficulty for an arbitrary $m<n$. But as there is the risk that the degree of notational complexity obscures the basically simple idea underlying the proof, we prefer to give the detailed calculation only for the case $m=2$ and hope to convince the reader that at every step of the reasoning one could replace the number 2 by an arbitrary m. For $m=2$ we have

$$\partial_{p_i^\alpha}\partial_{p_j^\beta}F(E,P)$$
$$=\partial_{P^\alpha}\partial_{p^\beta}F(E,P)+\partial_E\partial_{P^\beta}F(\cdots)\cdot\partial_{p_i^\alpha}\epsilon(p_i)$$
$$+\partial_E\partial_{P^\alpha}F(\cdots)\cdot\partial_{p_j^\beta}\epsilon(p_j)$$
$$+\partial_E\partial_E F(\cdots)\cdot\partial_{p_i^\alpha}\epsilon(p_i)\cdot\partial_{p_j^\beta}\epsilon(p_j)$$
$$=\partial_{p_i^\alpha}\partial_{p_j^\beta}f_{\{\cdots\}}(p_i,p_j). \tag{3.22}$$

With 2 (and in general m) smaller than n we can vary E, P while keeping p_i,p_j fixed! Doing this we see that because the rhs of the second equality has to remain constant

$$\begin{aligned}&\partial_P\partial_P F(E,P)=\text{const},\\ &\partial_E\partial_P F(\cdots)=\text{const},\\ &\partial_E\partial_E F(\cdots)=\text{const},\end{aligned} \tag{3.23}$$

in other words,

$$F(E,P)=A_{\alpha\beta}P^\alpha\cdot P^\beta+B_\beta E\cdot P^\beta$$
$$+C\cdot E\cdot E+\text{lin. terms}+\text{const.}, \tag{3.24}$$

where now $A_{\alpha\beta},B_\beta,C,\ldots$ are constants. For $f_{\{\cdots\}}(p_i,p_j)$ we have

$$f_{\{\cdots\}}(p_i,p_j)=A_{\alpha\beta}(p_i^\alpha p_i^\beta+p_i^\alpha p_j^\beta+p_i^\alpha p_j^\beta+p_j^\alpha p_j^\beta)$$
$$+B_\beta(\epsilon_i p_i^\beta+\epsilon_i p_j^\beta+\epsilon_j p_i^\beta+\epsilon_j p_j^\beta)$$
$$+C(\epsilon_i^2+2\epsilon_i\epsilon_j+\epsilon_j^2)$$
$$+\text{lin. terms}+\text{const.} \tag{3.25}$$

This proves the theorem.

In concluding this section we want to give special emphasis to the following observation which can be extracted

from the above proof.

Observation: $G_4|M = \partial_E F$, $\mathbf{G}|M = \partial_P F$, which shows (cf. Theorem 1 above) that G_4, $\mathbf{G}$ are in fact invariants being directly related to F itself!

IV. THE PHYSICAL SIDE OF THE PROBLEM

We have now to discuss the physical soundness of the crucial assumption being made in connection with scattering invariants of the first kind, namely that the possible scattering events are assumed to cover a full *open* neighborhood U on M. We start again with the simplest case, two particle scattering in momentum space. Assuming $\epsilon(p) = p^2$ $(m = 1)$, $M \subset \mathbb{R}^{12}$ is given by

$$p_1 + p_2 - p_1' - p_2' = 0, \quad p_1^2 + p_2^2 - p_1'^2 - p_2'^2 = 0,$$

i.e., M has dimension 8. The ingoing momenta p_1, p_2 can be freely chosen, which yields six degrees of freedom.

The two missing local coordinates on the manifold M can be found as follows. The asymptotical kinematics is described by $(t \to -\infty)$

$$x_i^0(t) = p_i \cdot t + x_i^0.$$

For a rotational symmetric pair potential scattering in the center of mass system takes place in a fixed plane $[(x_1 - x_2) \cdot (x_1 \times \dot{x}_1 + x_2 \times \dot{x}_2) = (x_1 - x_2) \cdot L = (\dot{x}_1 + \dot{x}_2)(x_1 \times x_2)$; with $\dot{x}_1 + \dot{x}_2 = 0$ we have $(x_1 - x_2) \cdot L = 0]$. The outgoing momenta p_1', p_2' are then uniquely given (at least locally) for given ingoing momenta p_1, p_2 by fixing the relative position at time zero, i.e.,

$$d := |x_1(0) - x_2(0)| \quad \text{and} \quad \theta := (x_1(0) - x_2(0)) \cdot p_1(0), \tag{4.1}$$

where d is the distance and θ is the "angle" between the *interacting* particles at $t = 0$. These two paramenters can be independently varied (at least for non-nasty potentials) via the initial conditions (x_1^0, x_2^0). Then d and θ can be used as local coordinates on M spanning together with (p_1, p_2) a full local coordinate system.

Thus we see that for two particle scattering and physically well-behaved potentials the preassumption of the existence of an open neighborhood U on M where concrete scattering takes place seems to be sound. Similar reasoning can be used for $n > 2$ particles in the case of a pure momentum dependence. But note that in any case x_{in}^1, x_{in}^2 are related to x_1^0, x_2^0 via the Möller transformation Ω_+, which is in general not simple. That means that the above reasoning, i.e., that by varying x_1^0, x_2^0 we can appropriately vary $x_{\text{in}}^1, x_{\text{in}}^2$ and hence p_1', p_2', is physically plausible but not mathematically proved. On the one side one can prove this for a large class of potentials, on the other there may be potentials where this does not hold, e.g., that by varying x_1^0, x_2^0 we get only a one-dimensional set of (p_1', p_2') for fixed ingoing momenta (p_1, p_2) s.t. U would have a dimension smaller than M itself. This is an interesting question which deserves a separate investigation.

The situation is *completely* different for more general invariants, depending on momenta *and* positions. Within the regime of classical nonrelativistic point mechanics there are ten *a priori* conservation laws, i.e., besides energy momentum, $L = \Sigma_i x_i(t) \times p_i$ and center of mass $S = \Sigma S_i(t)$, $S_i(t) = m_i x_i(t) - p_i \cdot t$. For the free motion this reduces to $\Sigma_i m_i x_i^0$. There are a couple of subtleties concerning the structure of the manifold M in this general case which will be discussed in the next chapter.

It will turn out that after certain modifications, M, defined by the above-mentioned conservation laws, is a $(12n - 10)$-dimensional set in $\mathbb{R}^{6n} \times \mathbb{R}^{6n}$. In contrast, however, to the pure momentum case, by fixing the initial conditions of the ingoing particles the initial conditions of the outgoing particles are uniquely given. That is, the manifold of *physical interest*, M_p, has only $6n$ dimensions, i.e., we have the following lemma.

Lemma 2: M_p, the manifold given by the set of pairs in $\mathbb{R}^{6n} \times \mathbb{R}^{6n}$: $\{x^0 p; S(x^0 p)\}$, $x^0 = (x_1^0, \ldots, x_n^0)$, etc., S viewed as a map: $\mathbb{R}^{6n} \to \mathbb{R}^{6n}$, is a true submanifold of the manifolds M defined by the conservation laws. The dimensions are $6n < 12n - 10$ for $n \geqslant 2$.

This shows that there is *no* chance to cover a full open neighborhood $U \subset M$ with real scattering processes for a fixed given interaction potential. Before we discuss the possible consequences of this fact we would like to make an aside about the use of cluster properties in this context.

Definition 6: We say the scattering transformation S_n (i.e., for n particles) clusters if the following holds: with $\inf_{j \neq i_0} |x_{i_0} - x_j| \to \infty$ for each position x_{i_0} we have

$$S_n(x_1 p_1, \ldots, x_{i_0} p_{i_0}, \ldots, x_n p_n) \to S_{n-1}(x_1 p_1, \ldots, x_{i_0} p_{i_0}, \ldots, x_n p_n) \times S_1(x_{i_0} p_{i_0}), \tag{4.2}$$

where

$$S_1(x_{i_0} p_{i_0}) = (x_{i_0}' p_{i_0}') = (x_{i_0} p_{i_0}).$$

That is, one can shift one of the ingoing particles to infinity s.t. in the limit it is not scattered at all. As is well known this cluster property is connected with the range of the interaction. Long range potentials have to be treated by a modified approach.

If we are in a situation where (4.2) holds we can proceed as follows. Restricting ourselves for simplicity for the moment to additive invariants we simply proceed by induction starting from $n = 2$. Assuming that for $n = 2$ we can, e.g., prove a certain structure of the collision invariants we treat the case $n = 3$ by shifting $|x_3^0|$ (resp. $|x_1^0|$, $|x_2^0|$) to ∞. Both for the two particle cluster and for the remaining single particle one we can employ the already proved result. We get the corresponding result for $n = 3$ by shifting particle (1) [resp. (2), (3)] back from infinity to their original positions, thus proceeding from an arbitrary $n - 1$ to n.

That is, in some cases one can reduce the analysis to the slightly simpler case $n = 2$. But even in this case the dimensions of M, M_p differ by 2 as long as the interaction potential is kept fixed. We will show in the next chapter that for collision invariants with $F(s,p) - F(s',p')$ vanishing on U *open* in M results similar to the previous ones can be proved $[s = \{s_i\} = \{m_i x_i^0(t) - p_i \cdot t\} = \{m_i x_1^0\}]$. On the other hand, it can now happen that the manifold M_F, defined by F, hits M transversally s.t.

$M_F \cap M$ contains no U open in M but

$$M_p \subset M_F \cap M \text{ locally.} \tag{4.3}$$

This implies in particular that one *cannot* decide by analyzing the scattering results whether F is an invariant of the first or second kind. As was argued after Definition 4, Sec. II, this may have important consequences. If $M_F \cap M$ has a lower dimension than M there may exist *additional* hidden symmetries being related to the corresponding transversal local coordinates defining $M_F \cap M$, that is, symmetries that show only up on M_p. Whether M_p can in particular support additional *additive* invariants is then a subtle question which depends on whether the detailed structure of M_p and M_F allows for an embedding $M_p \subset M_F$ locally in this special case (due to the assumed additivity M_F is relatively "flat," cf. Ref. 14).

Remarks: As to the use of cluster properties of the S matrix in this context we would like to add the following remark. Buchholz kindly informed us that the observation that things become simpler if one exploits the spacelike cluster properties of S was already made by the authors of Ref. 17 a couple of years ago without being published. It is an important tool in their paper.[17] Unfortunately we were not aware of this fact.

As a last point to mention, in the special case of additive conservation laws, the as yet unpublished results of Ref. 15 may have a certain bearing on the discussion of this chapter. By exploiting what we called above the relative "flatness" of the manifold M_F in the case of additive invariants one can possibly prove various results without assuming that certain sets on M are open.

V. THE CASE OF GENERAL COLLISION INVARIANTS

Discussion of the case of general invariants of the S transformation, depending on positions, momenta, and the time, needs more care. In a first step we have to define a manifold M adapted to our purpose. Since $\Sigma x_i(t) \times p_i = \Sigma x_i^0 \times p_i$, $\Sigma m_i x_i(t) - p_i t = \Sigma m_i x_i^0$ for free paths we can write the ten conservation laws in the following way:

$$\begin{aligned} &\sum p_i - \sum p_i' = 0, \\ &\sum \epsilon_i(p_i) - \sum \epsilon_i(p_i') = 0, \\ &\sum x_i(t) \times p_i - \sum x_i'(t') \times p_i' = 0, \\ &\sum s_i(t) - \sum s_i'(t') = 0, \end{aligned} \tag{5.1}$$

where $t \neq t'$ in general and $x_i(t) = x_i^0 + p_i/m_i \cdot t$.

Remark: To be concrete we discuss only the case of nonrelativistic point mechanics. In case of another type of mechanics the conservation of center of mass has to be expressed differently. But no step in our calculations depends actually on the concrete form of the conservation law of center of mass or of the functional dependence $\epsilon(p)$.

It is a simple but important observation that the various time dependencies of the quantities in (5.1) are only a pseudocomplication. In a first step we rewrite the angular momentum conservation law this way:

$$\sum s_i(t) \times p_i - \sum s_i'(t') \times p_i' = 0, \tag{5.2}$$

since $p_i \times p_i = 0$. In a second step we consider the problem in a new space, i.e., the space spanned by the $\{s_i, s_i', p_i, p_i'\}$. We forget about the time coordinates t, t' and observe that (5.1), (5.2) define a $(12_n - 10)$-dimensional manifold M in $\mathbf{R}^{6n} \times \mathbf{R}^{6n}$, spanned by the coordinates $\{s_i p_i; s_i' p_i'\}$.

Definition 7: M is defined by the relations

$$\begin{aligned} &\sum p_i - \sum p_i' = 0, \\ &\sum \epsilon_i(p_i) - \sum \epsilon_i(p_i') = 0, \\ &\sum s_i \times p_i - \sum s_i' \times p_i' = 0, \\ &\sum s_i - \sum s_i' = 0 \end{aligned}$$

in $\mathbf{R}^{6n} \times \mathbf{R}^{6n}$, coordinates: $\{s_i, p_i; s_i' p_i'\}$.

In a next step we show that collision invariants $F(x(t), p, t)$ are automatically functions of s, p.

Lemma 3: A general collision invariant $F(x(t), p, t)$ is a function of s, p, that is $F(x(t), p, t) \hat{=} F(s, p)$.

Proof: The proof is simple. We have

$$\begin{aligned} F(\mathbf{x}(t), p, t) &= F(x^0, p, 0) = F(\{x_i - p_i/m_i \cdot t\}, p) \\ &= F(s, p) \end{aligned} \tag{5.3}$$

(identifying the functions for simplicity). We can then prove the following theorem.

Theorem 4: Let $F(\{x_i(t), p_i\}, t) \in C^1$ be an invariant of the first kind, i.e., $F(s, p) - F(s', p') \equiv 0$ on an open neighborhood $U \subset M$, M defined by Definition 7, then it fulfills the structural relation:

$$\begin{aligned} &F(s,p) - F(s',p') \\ &= G^{\nu} \cdot \left(\sum p_i - \sum p_i' \right)^{(\nu)} \\ &\quad + G_4 \cdot \left(\sum \epsilon_i(p_i) - \sum \epsilon_i(p_i') \right) \\ &\quad + H_{\nu} \cdot \left(\sum x_i(t) \times p_i - \sum x_i'(t') \times p_i' \right)^{(\nu)} \\ &\quad + K_{\nu} \cdot \left(\sum s_i(t) - \sum s_i'(t') \right)^{(\nu)}, \end{aligned} \tag{5.4}$$

with $G^{\nu}, G_4, H_{\nu}, K_{\nu}$ in general functions of s, s', p, p'. Equation (5.4) holds on $\tilde{U} \supset U$, $\tilde{U}$ open in $\mathbf{R}^{6n} \times \mathbf{R}^{6n}$.

Proof: Employing Lemma 3 the proof is analogous to the one of Theorem 1. Note that $x_i(t) \times p_i = s_i(t) \times p_i = s_i \times p_i$ for free paths.

If F is only an invariant of the second kind, i.e., $M_F \cap M$ has no open neighborhood in M but $M_F \cap M_p$ contains an open set in M_p, we would get the following theorem, in general.

Theorem 5: With $M_F \cap M_p$ containing an open neighborhood $\hat{U} \subset M_p$ we have the corresponding relation on $\tilde{U} \supset \hat{U}$, $\tilde{U}$ open in $\mathbf{R}^{6n} \times \mathbf{R}^{6n}$:

$$\begin{aligned} &F(s,p) - F(s',p') \\ &\quad = \{\text{rhs of (5.5)}\} + \sum_i \alpha_i A_i, \quad i = 1, \ldots, 12n - 10 - 6n, \end{aligned} \tag{5.5}$$

with $\{\alpha_i\}$ functions of $\{s, p, s', p'\}$ and $\{A_i\}$ functions vanish-

ing *identically* on $\hat{U} \subset M_p$.

Proof: Most of the proof goes through as above. We only need the following additional lemma.

Lemma 4: Every submanifold of a manifold M is locally cut out by independent functions, i.e., it is the zero set of, e.g., $\{A_i\}$ in addition to the functions defining M itself.

Proof: See, e.g., Ref. 21.

Remark: The possible occurrence of the terms $\alpha_i A_i$ will, in general, destroy the simple structure given, e.g., in Theorem 3. Note that A_i need not even have the form $F_{A_i}(p,s) - F_{A_i}(p',s')$.

In the following we will restrict ourselves to invariants of the first kind. We then proceed as in Sec. III. Assuming again that F is twice differentiable we begin with differentiating with respect to s_i which turns out to be advantageous. We then restrict again the result to $U \subset M$ s.t. all the terms $(\Sigma p_i - \Sigma p_i')$,... vanish indentically. So we get

$$(\partial_{s_i} F(p,s))^{(\alpha)} | U = \epsilon_{\nu\alpha\beta} p_i^\beta \cdot H^\nu + K^\alpha \tag{5.6}$$

and

$$(\partial_{s_i} F - \partial_{s_j} F)^{(\alpha)} | U = \epsilon_{\nu\alpha\beta} H^\nu (p_i^\beta - p_j^\beta), \tag{5.7}$$

where ν, α, β, denote the components of the various three-vectors and with $\epsilon_{\nu\alpha\beta}$ the totally antisymmetric three-tensor. Note that H^ν does not depend on the particular i,j being chosen. Now we differentiate with respect to p_i, p_j, and get

$$(\partial_{pi} F(p,s))^{(\beta)} | U = G^\beta + \partial^\beta_{p_i} \epsilon_i(p_i) \cdot G^4 + \epsilon_{\nu\alpha\beta} s_i^\alpha \cdot H^\nu + K^\beta \tag{5.8}$$

and the analogous expression for the index $\{j\}$. Subtracting the two expressions we get rid of G^β and can isolate G^4. As in the pure momentum case we get explicit expressions for all the unknown functions $\{G_4, G_\beta, H_\beta, K_\beta\}$. As in Theorem 1, Sec. III, we see that all these functions are necessarily *scattering invariants* on $U \subset M$!

In the special case of additive invariants we get more detailed information. With $F(p,s) = \Sigma_i f_i(p_i,s_i)$ we get on the lhs of (5.7):

$$\partial_{s_i} f_i(p_i,s_i) - \partial_{s_j} f_j(p_j,s_j). \tag{5.9}$$

By the same reasoning as in Theorem 2, Sec. III, we see that the H_ν are constants [that is, by varying (i,j)]. Inserting this into (5.6) we see that the K_ν are constants. We then subtract the expressions (5.8) for the index i (resp. j) from one another, employing $H_\nu = \text{const}$, $K_\nu = \text{const}$. We get by the same token $G_4 = \text{const}$, $G_\nu = \text{const}$. That is, we wind up with the following theorem.

Theorem 6: Let $F(\{p_i,s_i\})$ be a general invariant of the *first* kind, and U be the corresponding neighborhood on the scattering manifold M defined in Definition 7. Furthermore, we assume F to be twice differentiable.

Then (i) F fulfills Eqs. (5.6)–(5.8) by which the unknown functions $\{G_4, G_\nu, H_\nu, K_\nu\}$ can be determined.

(ii) The $\{G_4, G^\nu, H_\nu, K_\nu\}$ are themselves scattering invariants on M, i.e.,

$$G_4(ps, p's') = G_4(ps) = G_4(p's') \text{ on } U \subset M. \tag{5.10}$$

(iii) In the case of an additive invariant, all these functions are *constant*.

We get

$$F(p,s) = \sum_i f_i(p_i,s_i) = G^\nu \cdot \Big(\sum p_i\Big)^{(\nu)} + G_4 \cdot \Big(\sum \epsilon_i(p_i)\Big) + H_\nu \cdot \Big(\sum x_i(t) \times p_i\Big)^{(\nu)} + K_\nu \cdot \Big(\sum s_i(t)\Big)^{(\nu)} + C, \tag{5.11}$$

that is, every additive invariant of the first kind is a superposition of the ten conserved quantities already known.

We want to conclude this chapter with the following theorem which is the analog to Theorem 3 in Sec. III in this general case.

Theorem 7: Let $F(p,s)$, an invariant of the first kind, be twice differentiable, $\partial_p \epsilon(p) \neq 0$ a.e., then the following holds.

(i) F is already a function of overall energy, momentum, angular momentum, center of mass, E,P,L,S, and we have, in particular,

$$\partial_E F = G^4, \quad \partial^\nu_P F = G^\nu, \quad \partial^\nu_L F = H^\nu, \quad \partial^\nu_S F = K^\nu.$$

(ii) If F is an m-particle observable with $m < n$ and $F \in C^m$, then the F (resp. the corresponding f) are at most polynomials of mth order in the variables $\{P^\alpha, E, L^\beta, S^\gamma\}$ (resp. $\{p_i, \epsilon_i, l_i, s_i\}$).

Proof: Take Eqs. (5.6)–(5.8). Choose, as in the proof of Theorem III, a new local coordinate system with E,P,L,S representing the first ten coordinates, $\zeta_{11} = p_2^3$, $\zeta_{12} = s_2^3$, etc., view F as a function of these new coordinates, and insert it into (5.6) and (5.8). We get

$$\begin{aligned} &\partial^\alpha_S F + \partial^\nu_L F \cdot \epsilon_{\nu\alpha\beta} p_i^\beta + \partial_\zeta F \cdot \partial^\alpha_{s_i} \zeta = \epsilon_{\nu\alpha\beta} p_i^\beta \cdot H^\nu + K^\alpha, \\ &\partial^\beta_P F + \partial_E F \cdot \partial^\beta_{p_i} \epsilon_i(p_i) + \partial^\nu_L F \cdot \epsilon_{\nu\alpha\beta} s_i^\alpha + K^\beta \\ &\quad = G^\beta + \partial^\beta_{p_i} \epsilon_i(p_i) \cdot G^4 + \epsilon_{\nu\alpha\beta} s_i^\alpha \cdot H^\nu + K^\beta. \end{aligned} \tag{5.12}$$

Choosing, in particular, $s_i^\alpha = s_1^1$, $s_j^\alpha = s_2^1$, $p_i^\beta = p_1^1$, $p_j^\beta = p_2^1$, we conclude with the help of expressions (5.7),...,

$$\partial^\nu_L F = H^\nu, \quad \partial^\nu_S F = K^\nu, \quad \partial^\nu_P F = G^\nu, \quad \partial_E F = G^4, \tag{5.13}$$

which shows, as in Theorem III, that F is already a function of E,P,L,S! The second part of the theorem will be proved exactly along the same lines as in the proof of Theorem III.

Summary and outlook: Since Sec. VI will supply us only with an explicit example of an (even) additive invariant of the second kind for a, however, very special potential, we want to briefly sum up what we have shown above and where future work has to set in.

(i) We have completely classified the scattering invariants depending only on the momenta of the particles in Theorem 3, viz., they are all functions of overall energy and momentum. The same analysis applies to translation covariant invariants in quantum theory and quantum field theory.

(ii) In the case of the more general invariants, depending also on the positions of the particles and the time, we found that they can be grouped into two different classes. For invariants of the first kind we could show again that they are functions of, now, overall energy, momentum, angular

momentum, and center of mass. The two classes are distinguished by a geometric property, viz., (1) M_F contains M locally, or (2) M_F intersects M transversally. Since $\dim(M_F) = 12n - 1 > \dim(M) = 12n - 10$, both situations can occur. [In order not to overburden the text we discussed the case (ii) only within the regime of classical mechanics.]

(iii) In case F is an m-particle invariant with $m < n$ it could even be shown that F is a polynomial of at most mth order in E,P,L,S in situation (i). We think that the restriction $m < n$ is not superfluous since it might well occur for some special n_0 that there are invariants depending on all n_0 particles that cannot be embedded in spaces with $n > n_0$! (A possible example might be the Runge–Lenz vector.)

(iv) Future work has to deal with these invariants of the second kind mentioned in (ii) (2). In that case the geometry of the intersection of M_F and M needs a careful study. The corresponding *nonlocal* invariants in quantum field theory that are not translation covariant are also studied elsewhere. We would like to mention in this context that it may turn out to be an advantage that our formalism is wide enough to incorporate also charges not commuting with the S matrix. Objects like these may also exist in classical mechanics since invariants of motion (i.e., commuting with H) do not(!) necessarily commute with the S matrix. In that case more is needed (somewhat sloppily: they should comute as well with H_0 in the limit $|t| \to \infty$). Possibly some of the initial conditions of classical mechanics are just of this kind.

VI. AN EXAMPLE OF AN INVARIANT OF THE SECOND KIND

It is obvious that the notion of an invariant of the second kind is not purely academic. We will see that there exist even additive examples of this type. On the other side, the structure of the manifolds M_p, M, M_F (F the invariant) and their mutual intersections are not easy to visualize so that it is quite helpful to get indirect evidence by means of, e.g., Theorem 6.

By Theorem 6 we know that every additive invariant F s.t.

$$M_F \cap M \supset U \quad (U \text{ open in } M),$$
$$M_F := \text{zero set of } F(p,s) - F(p',s') \quad \text{in } \mathbb{R}^{6n} \times \mathbb{R}^{6n}, \tag{6.1}$$

holds, in other words M being locally contained in M_F, is necessarily of the form (5.12), that is, with constant coefficients G,H,K,C. If for a certain given pair interaction V we can show that there is an additive invariant which is not of the form (5.12) it is necessarily of the second kind, that is,

$$M_F \text{ hits } M \text{ transversally},$$
$$M^F \cap M \text{ contains no open } U \text{ but}$$
$$M_p \subset M_F \text{ locally, where } M_p := \{(p,s); S(p,s)\}. \tag{6.2}$$

Now take in the two-body case the potential to be $V(r) = C \cdot r^{-2}$. One knows that the so-called time delay T is zero in this case. (For the definition of time delay cf., e.g., Refs. 4 and 6, it can also be found implicitly in Chap. 14 of Ref. 1. See also Appendix B in Ref. 14.) We have

$$T = (s \cdot p - s' p')/p^2, \tag{6.3}$$

with $s,p,\ldots$, taken in the center of mass system. Calculating T by using the more explicit expression for T with the potential in it (see the above references) we observe that $T = 0$ for $V = c \cdot r^{-2}$, i.e.,

$$s_1 \cdot p_1/m_1 + s_2 \cdot p_2/m_2 \text{ is a scattering invariant on } M_p. \tag{6.4}$$

On the other side this invariant is not linearly expressible as a superposition of P,E,S,L. So it is an explicit example for which the preassumption of the existence of an open neighborhood U on M, where $F(s,p) = F(s',p')$ holds, is not fulfilled.

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Uniqueness of the metric from the Weyl and energy-momentum tensors

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It is shown that for a general space-time in Einstein's theory (with the term "general" being precisely defined) the Weyl tensor and energy-momentum tensor determine the metric up to a constant conformal factor. One of the conclusions may be interpreted as a generalization of the well-known Brinkmann theorem characterizing *pp* waves *in vacuo*.

I. INTRODUCTION

Let (M, g) be a space-time manifold where M is a real, smooth, four-dimensional, connected, Hausdorff manifold and g a smooth Lorentz metric on M with signature $(-,+,+,+)$. The usual notation will be used so that the components of the curvature tensor, Ricci tensor, Weyl tensor, and Ricci scalar in some coordinate system in M are denoted, respectively, by $R^{a}{}_{bcd}$, $R_{ab}\,(\equiv R^{c}{}_{acb})$, $C^{a}{}_{bcd}$, and $R\,(\equiv R_{ab}g^{ab})$, where the g_{ab} are the metric tensor components. The decomposition of the curvature tensor into its self-dual and anti-self-dual parts is

$$R^{a}{}_{bcd} = C^{a}{}_{bcd} + \tfrac{1}{6}RG^{a}{}_{bcd} + E^{a}{}_{bcd}\,, \tag{1}$$

where

$$\begin{aligned} &E^{a}{}_{bcd} = \tilde{R}^{a}{}_{[c}g_{d]b} + \tilde{R}_{b[d}\,\delta_{c]}{}^{a}\,,\\ &\tilde{R}_{ab} = R_{ab} - \tfrac{1}{4}Rg_{ab}, \quad G^{a}{}_{bcd} = \delta^{a}_{[c}g_{d]b}\,, \end{aligned} \tag{2}$$

and Einstein's equations are

$$G_{ab} \equiv R_{ab} - \tfrac{1}{2}Rg_{ab} = 8\pi T_{ab}\,, \tag{3}$$

where the G_{ab} and T_{ab} are the components of the Einstein tensor and the energy-momentum tensor, respectively, and a square bracket denotes the usual skew symmetrization.

It has recently been shown that if the curvature tensor of space-time, with components $R^{a}{}_{bcd}$, is given (and assumed to arise from some Lorentz metric on M) then the number of other Lorentz metrics on M that yield the same curvature components is severely limited.[1-3] The following results, taken from Ref. 2, will be required in what is to follow. They are stated here in a slightly more general form than in Ref. 2.

(i) Suppose $\phi: M \to \mathbb{R}$ is a positive, smooth function and let g and $g' \equiv \phi g$ be smooth Lorentz metrics on M with the same curvature tensor (that is, the components $R^{a}{}_{bcd}$ are the same for both metrics in any coordinate system). Suppose also that this curvature tensor is nonflat in the sense that it does not vanish over an open subset of M. Then the Bianchi identities for g and g' lead to

$$\phi_{,a}R^{a}{}_{bcd} = 0 \tag{4}$$

at each point of M (where a comma denotes a partial derivative) and so, provided the equation $k_aR^{a}{}_{bcd} = 0$ has no solution for a nonzero one-form k over an open subset of M, ϕ is necessarily constant on M. The symmetric connections arising from g and g' are then equal.

(ii) Suppose g and g' are smooth Lorentz metrics on M with the same Weyl tensor components $C^{a}{}_{bcd}$. Suppose also that the Weyl tensor is nowhere of Petrov type N in the sense that the equation $k_aC^{a}{}_{bcd} = 0$ has no solution for a nonzero one-form k over an open subset of M. Then g and g' are conformally related.

II. BRINKMANN'S THEOREM

In 1925, Brinkmann[4] proved a theorem, a special case of which has become well known in general relativity.[5] This special case says that if g and g' are conformally related, nonflat, vacuum metrics on a space-time M then either the conformal factor is constant or g and g' are each *pp*-wave metrics. A generalization of this theorem will now be given when the vacuum condition is dropped.

Suppose $\phi: M \to \mathbb{R}$ is a positive smooth function and that g and $g' \equiv \phi g$ are nonflat Lorentz metrics on a space-time M. Using primed and unprimed symbols in an obvious way, the vacuum condition is replaced by the statement that the corresponding Einstein tensors are equal, so that in any coordinate system $G'_{ab} = G_{ab}\,[\Leftrightarrow T'_{ab} = T_{ab}$ from (3)$]$. It then follows that the algebraic (Segrè type) structure of T_{ab} with respect to g_{ab} is the same as that of T'_{ab} with respect to g'_{ab} and that $R'_{ab} = R_{ab}$, $R' = \phi^{-1}R$, and $\tilde{R}'_{ab} = \tilde{R}_{ab}$. Equation (2) then implies that $E'^{a}{}_{bcd} = E^{a}{}_{bcd}$ and $G'^{a}{}_{bcd} = \phi G^{a}{}_{bcd}$. Also, the fact that g and g' are conformally related gives $C'^{a}{}_{bcd} = C^{a}{}_{bcd}$ and this, together with the relation $g' = \phi g$, shows that the algebraic (Petrov) types of (M, g) and (M, g') are the same. Equation (1) then gives $R'^{a}{}_{bcd} = R^{a}{}_{bcd}$. This result, together with result (i) in Sec. I leads to the following theorem which is the first generalization of Brinkmann's theorem and was given in Ref. 6.

Theorem 1: Let g and g' be conformally related nonflat Lorentz metrics on M whose Einstein tensors are equal. Then the corresponding curvature components $R^{a}{}_{bcd}$ are equal and, if the equation $k_aR^{a}{}_{bcd} = 0$ has no solution for a nonzero one-form k over an open subset of M, the conformal factor is constant and the symmetric connections arising from g and g' are equal.

A related result has been given by Ihrig.[7] A simple consequence of Theorem 1 and result (ii) in Sec. I is the following theorem.[6]

Theorem 2: Suppose a space-time (M, g) has the property that there are no nonzero solutions for the one-form k of the equations $k_aR^{a}{}_{bcd} = 0$ or $k_aC^{a}{}_{bcd} = 0$ over an open subset of M. Then, in any coordinate domain, the components $C^{a}{}_{bcd}$ and G_{ab} uniquely determine the components $R^{a}{}_{bcd}$

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and the metric tensor g is determined up to a constant conformal factor. The symmetric connection on M is then uniquely determined.

A stronger generalization of Brinkmann's theorem can now be given. Before this is done it is recalled that, loosely speaking, a *pp*-wave metric can be characterized as a nonflat vacuum space-time admitting a nowhere zero, covariantly constant (necessarily null) vector field.[5] Further, if g and $g' \equiv \phi g$ are nontrivially conformally related *pp*-wave metrics (in the sense that ϕ is not a constant function on M) then the covariantly constant null vector fields associated with g and g' which arise on M and the vector fields $\phi_{,a} g^{ab}$ and $\phi_{,a} g'^{ab}$ are parallel.

Theorem 3: Let $\phi: M \to \mathbf{R}$ be a positive smooth function and g and $g' \equiv \phi g$ be conformally related, nonflat Lorentz metrics on M whose Einstein tensors are equal. Then either (i) ϕ is constant on M; (ii) (M, g) and (M, g') each admit a nowhere zero, covariantly constant null vector field and any geodesic in either of these space-times, not lying in the hypersurfaces $\phi = \text{const}$, is incomplete; or (iii) the normal curves to the surfaces $\phi = \text{const}$ are incomplete non-null geodesics with respect to both g and g', the space-times (M, g) and (M, g') each admit a non-null, nowhere zero, gradient homothetic Killing vector field and local coordinates may be chosen about any point of M such that g takes the forms given in (7) and (9) below.

The proof begins by using the condition $R'_{ab} = R_{ab}$ (from the proof of Theorem 1) and the standard relation between the Ricci tensor components of two conformally related metrics (see, for example, Ref. 8). One easily finds that if $V = \phi^{-1/2}$ then

$$V_{;ab} = \tfrac{1}{4}\gamma g_{ab} \quad (\gamma = V_{;ab} g^{ab}), \tag{5}$$

where a semicolon denotes a covariant derivative with respect to g. The proof of Theorem 1 also shows that g and g' have the same curvature tensor components $R^{a}{}_{bcd}$ and so Eq. (4) yields the relation $V_{,a} R^{a}{}_{bcd} = 0$. This together with the relation $4V_{;a[bc]} = g_{a[b}\gamma_{,c]}$ obtained from (5) and the Ricci identity with respect to g then show that $\gamma_{,a} = 0$ and so γ is constant on M since M is connected. Next, the proof of Theorem 1 also shows that $\phi R' = R$ and then the standard relation between the Ricci scalars of two conformally related metrics (see, for example, Ref. 8) leads to

$$2V^{-1} V_{,a} V_{,b} g^{ab} = V_{;ab} g^{ab} \quad (= \gamma). \tag{6}$$

If $\gamma = 0$ on M Eq. (5) shows that $V^a \equiv V_{,b} g^{ab}$ is a covariantly constant vector field on (M, g) and then Eq. (6) shows that either $V^a = 0$ on M (and so V, and hence ϕ, is constant on M) or V^a is a nowhere zero, covariantly constant, null vector field on (M, g) [and which, after an appropriate scaling, gives rise to one on (M, g')]. It then follows, for example, in (M, g) that if c is a geodesic with affine parameter τ not lying in the hypersurface $\phi = \text{const}$ then $dV/d\tau$ is equal to a nonzero constant along c because of the relation $V_{a;b} = 0$. Since V is a positive function on M, c is, therefore, incomplete. If $\gamma = \text{const} \neq 0$ on M, Eqs. (5) and (6) show that V^a is a proper, gradient, nowhere zero, homothetic Killing vector field on (M, g) [and a similar vector field arises on (M, g')] and it is clear that the paths of V^a are everywhere spacelike or everywhere timelike geodesics with respect to both g and g'. If one selects any affine parameter τ along any of these geodesics in (M, g) one finds that $(d/d\tau)(|\kappa|^{1/2})$ is constant, where $\kappa = V^a V^b g_{ab}$. This means that κ will become zero after a finite affine parameter distance along the geodesic in a certain direction. However, Eq. (6) forbids $\kappa = 0$ because $\gamma \neq 0$ and so the geodesic is incomplete. Now consider the case when V^a is timelike. By constructing local Gaussian coordinates about any point based on the geodesic flow V^a and using the fact that V^a is a gradient, homothetic Killing vector field [that is, using only Eq. (5) with γ a nonzero constant] one can arrange the metric g in the form (cf. Ref. 9)

$$ds^2 = -dt^2 + t^2 h_{\alpha\beta}\, dx^\alpha\, dx^\beta, \tag{7}$$

where the x^α are local coordinates in the hypersurface $t = \text{const}$ and where the $h_{\alpha\beta}$ are independent of the affine parameter t along the geodesic flow. One then finds that V is a function of t only and that

$$\frac{d^2 V}{dt^2} = V_{a;b}\delta^a_0 \delta^b_0 = -\frac{1}{4}\gamma \quad \left(\Rightarrow V = -\frac{1}{8}\gamma t^2 + \alpha t + \beta\right), \tag{8}$$

with α and β constants. Use of Eq. (5) again then shows that $\alpha = 0$. Then Eq. (6) implies that $\beta = 0$ and so $V = -\frac{1}{8}\gamma t^2$. A similar situation occurs when V^a is spacelike. Instead of (7) one has, in an obvious notation,

$$ds^2 = dx^2 + x^2 h'_{\alpha\beta}\, dx^\alpha\, dx^\beta, \quad V = \tfrac{1}{8}\gamma x^2, \tag{9}$$

where the $h'_{\alpha\beta}$ are the components of a three-dimensional Lorentz metric in the hypersurfaces $x = \text{const}$ and are independent of x. This completes the proof.

Conversely if one has a metric g of the form (7) then the function $V = -\frac{1}{8}\gamma t^2$ satisfies (5) and (6) and the metrics g and ϕg, where $\phi^{-1/2} = V$ have the same energy-momentum tensor and hence the same curvature tensor.

Using result (ii) of Sec. I and Theorem 3 one has the following theorem.

Theorem 4: Let (M, g) be a space-time with the following properties: (i) (M, g) is geodesically complete; and (ii) the Weyl tensor components $C^{a}{}_{bcd}$ in any coordinate domain are such that there are no nonzero solutions for the one-form k of the equation $k_a C^{a}{}_{bcd} = 0$ over an open subset of M. Then in any coordinate domain the components $C^{a}{}_{bcd}$ and G_{ab} uniquely determine the metric g up to a constant conformal factor.

The vacuum *pp* waves can also be characterized as those nonflat vacuum metrics admitting a covariantly constant (necessarily null) bivector field or as those nonflat vacuum metrics whose curvature tensor is complex recurrent.[5] They are of Petrov type N. It is perhaps of interest to examine which of these properties is possessed by those metrics occurring in part (ii) of Theorem 3, that is, those metrics admitting a nowhere zero, covariantly constant, null vector field l. The Ricci identity and Eqs. (1) and (2) show that the Weyl tensor is either zero or else algebraically special with repeated principal null direction l at each point of M. It seems that all algebraically special types can occur. However, if the Weyl tensor is type III at any point of M then the dominant energy conditions (as given, for example, in Ref.

10) fail at that point. This is because the type III requirement on the Weyl tensor expressed in terms of the Bel criteria[11] together with the relations $R_{abcd}l^d = 0$ and $R_{ab}l^b = 0$ and Eqs. (1) and (2) show that $R = 0$ and that the Ricci tensor has Segrè type $\{(31)\}$ with zero eigenvalue.[12] The connection between the Petrov type and the Segrè type of the energy-momentum tensor on the basis of the relation $R_{abcd}l^d = 0$ is given in Ref. 3. If the Weyl tensor is of Petrov type N or 0 at any point of M then a similar calculation to that described above shows that again $R = 0$ at that point and the Ricci tensor, if nonzero, is of Segrè type $\{(211)\}$ with zero eigenvalue, taking the form $R_{ab} \propto l_a l_b$. The converse is also true. If the type N condition holds over an open subset U of M a differentiation of the equation $\overset{+}{C}_{abcd}l^d = 0$, where $\overset{+}{C}_{abcd}$ is the complex self-dual Weyl tensor, shows that the Weyl tensor is complex recurrent ($\overset{+}{C}_{abcd;e} = \overset{+}{C}_{abcd}p_e$ for some one-form p). A similar argument shows that, whatever the Petrov type, any complex, self-dual null bivector F_{ab} with principal null direction l is also complex recurrent, $\overset{+}{F}_{ab;c} = \overset{+}{F}_{ab}q_c$ for some one-form q. When the Petrov type is N or 0 over an open subset U of M, the algebraic restrictions on C_{abcd} and R_{ab} show that $\overset{+}{F}_{ab;[cd]} = 0$.[13] Hence in these cases q is locally a gradient, $q_a = \psi_{,a}$ for some differentiable function ψ, and $e^{-\psi}\overset{+}{F}_{ab}$ is a constant, complex, null bivector. As expected, these cases show the closest similarity to the *pp* waves.

For those metrics occurring under the conditions of part (iii) of Theorem 3 [metrics (7) and (9)] one can establish a correspondence between the Petrov type, the algebraic (Segrè) type of the space-time Ricci tensor, and the algebraic type of the intrinsic Ricci tensor in the hypersurfaces $V = \text{const}$. This correspondence is particularly easy when these hypersurfaces are spacelike. In this case it turns out that at each point the Petrov type is I, D, or 0. The respective Segrè types for the Ricci tensor are $\{1,111\}$, $\{1,1(11)\}$, or $\{1,(111)\}$ (where in each case further degeneracies involving the timelike eigenvalue only are permitted) and for the intrinsic hypersurface Ricci tensor, $\{111\}$, $\{1(11)\}$, or $\{(111)\}$. This follows in a straightforward way from the Gauss equation connecting the space-time curvature and the intrinsic hypersurface curvature, the relation $V_{,a}R^a{}_{bcd} = 0$, and the table in Ref. 3. The hypersurfaces $V = \text{const}$ are, incidentally, umbilical hypersurfaces each with constant mean curvature.

The above discussion concerns those special cases when the prescription of the Weyl tensor and Einstein (or energy-momentum) tensor, in the sense of Theorem 2, does not determine the metric tensor up to a constant conformal factor. However, it was remarked in Ref. 6 that, in the general case, one would expect the conclusions of Theorem 2 to hold. This can be made precise in the following way. Let L be the set of C^r Lorentz metrics on M ($r \geqslant 3$) and let $\Gamma^r(L)$ denote the topological space comprising this set together with the Whitney C^r topology (for further details on jet bundles and the Whitney topologies see Ref. 14). It has been shown in Ref. 15 that there exists an open, dense subset W of $\Gamma^r(L)$ such that for each $g \in W$ there are no nonzero solutions for the one-form k of the equations $k_a R^a{}_{bcd} = 0$ or $k_a C^a{}_{bcd} = 0$ associated with g at any $p \in M$. This result, together with Theorem 2, leads to the final theorem which will be stated, somewhat informally, as the following.

Theorem 5: It is generic for the Weyl tensor and Einstein (or energy-momentum) tensor on M to determine the metric on M up to a constant conformal factor and to determine the connection on M uniquely.

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Lorentz invariance and the equivalence of metric, spinor, and frame field concomitants

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Any theory constructed out of the metric tensor and its derivatives can also be regarded as a theory constructed out of a frame field and its derivatives. In general, the converse is not true. It is shown that with the additional assumption that the theories are Lorentz invariant the converse *is* true. Theories involving the metric spinor and its derivatives are then included in this equivalence and the various interrelationships are studied.

I. INTRODUCTION

In the study of concomitants in relativity,[1] there are three objects that can be used to represent the gravitational field: (i) the metric tensor g_{ij}, $i,j = 1,...,4$; (ii) the frame field (orthonormal tetrad or vierbein) h_i^{α}, $\alpha = 1,...,4$; or (iii) the spin-tensor[2] $\sigma_{iAX'}$, $A,X' = 1,2$. Here, lowercase Latin indices signify space-time components, lowercase Greek indices signify frame components, and uppercase Latin indices signify spinor components. By virtue of the definition

$$\sigma_{iAX'} \equiv h_i^{\alpha}\sigma_{\alpha AX'} ,$$

where the $\sigma_{\alpha AX'}$ are the conventional Pauli spin matrices, any concomitant of h_i^{α} and its derivatives can be regarded as a concomitant of $\sigma_{iAX'}$ and the same number of its derivatives and vice versa. The relation between the metric and the frame field is

$$g_{ij} = h_i^{\alpha}h_j^{\beta}\eta_{\alpha\beta} , \tag{1.1}$$

where $\eta_{\alpha\beta} \equiv \mathrm{diag}(-1,-1,-1,1)$. Hence any concomitant of g_{ij} and its derivatives is a concomitant of h_i^{α} and its derivatives. However, the converse is not necessarily true, as can be seen by the vector

$$A_i \equiv h_{i|j}^{\alpha}h_{\alpha}^{j} , \tag{1.2}$$

where a vertical bar denotes covariant differentiation, i.e.,

$$h_{i|j}^{\alpha} \equiv h_{i,j}^{\alpha} - \{{}_i{}^k{}_j\}h_k^{\alpha} ,$$

where a comma denotes partial differentiation with respect to the local coordinate x^j and $\{{}_i{}^k{}_j\}$ is the Christoffel symbol of the second kind. Clearly,

$$A_i = A_i(h_j^{\alpha};h_{j,k}^{\alpha})$$

and yet A_i cannot be expressed as

$$A_i = A_i(g_{jk};g_{jk,h}) , \tag{1.3}$$

since the invariance identities[3] for such an A_i under a coordinate transformation imply that tensors of the form (1.3) vanish identically.[4]

We shall show that, in the more general case of second-order concomitants, there is an equivalence if, in addition, one assumes that the concomitant is invariant under a proper orthochronous Lorentz transformation, i.e.,

$$h'^{\alpha}_i = \mathcal{L}^{\alpha}_{\beta}h_i^{\beta} ,$$

where $\mathcal{L}^{\alpha}_{\beta}$ is a Lorentz matrix. Thus all three types of concomitants will be equivalent. Since A_i as given by (1.2) violates Lorentz invariance we see the need for this restriction to obtain the equivalence.

The proof of this result relies on the use of invariance identities,[3,5] which arise from the demand of Lorentz invariance. It is actually valid for a space of arbitrary dimension and signature. The group involved must necessarily preserve this signature, i.e., it consists of matrices $\mathcal{L}^{\alpha}_{\beta}$, $\alpha,\beta = 1,...,n$, such that

$$\eta_{\alpha\beta} = \mathcal{L}^{\mu}_{\alpha}\eta_{\mu\nu}\mathcal{L}^{\nu}_{\beta} ,$$

where $\eta_{\alpha\beta} \equiv \mathrm{diag}(\pm 1,\pm 1,...,\pm 1)$. We will call it the *signature group.*

There are two notable consequences of this result. The first is that the notion of gravity as a Lorentz gauge theory[6] is reinforced. The second is that it enables us to simplify the proofs of known results[7] and generate new ones, as will be shown in Sec. III.

II. EQUIVALENCE

We start with an arbitrary second-order concomitant of the frame field, i.e.,

$$A = A(h_i^{\alpha};h_{i,j}^{\alpha};h_{i,jk}^{\alpha}) .$$

It turns out that it does not matter how A transforms under a coordinate transformation, so all space-time indices are suppressed on A. In order to derive the invariance identities for A, it is convenient to coordinatize the signature group such that an element $\mathcal{L}^{\alpha}_{\beta}$ of the connected component of the identity can be expressed as

$$\mathcal{L}^{\alpha}_{\beta} = \exp(-u^{\alpha\gamma}\eta_{\gamma\beta}) ,$$

where $u^{\alpha\gamma}(x^i) = -u^{\gamma\alpha}(x^i)$ are the coordinates relative to a canonical chart of the first kind.[6,8] The invariance of A under a signature group transformation is expressed as

$$A(h'^{\alpha}_i;h'^{\alpha}_{i,j};h'^{\alpha}_{i,jk}) = A(h_i^{\alpha};h_{i,j}^{\alpha};h_{i,jk}^{\alpha}) . \tag{2.1}$$

The three invariance identities obtained by differentiating (2.1) with respect to $u^{\gamma\omega}{}_{,rs}$, $u^{\gamma\omega}{}_{,r}$, and $u^{\gamma\omega}$ and then evaluating at the identity transformation $u^{\gamma\omega} = 0$, reduce to

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$$\frac{\partial A}{\partial h^{\alpha}_{i,rs}}\delta^{\alpha\theta}_{\gamma\omega}\eta_{\theta\beta}h^{\beta}_{i}=0\,, \tag{2.2a}$$

$$\frac{\partial A}{\partial h^{\alpha}_{i,r}}\delta^{\alpha\theta}_{\gamma\omega}\eta_{\theta\beta}h^{\beta}_{i}+\frac{2\,\partial A}{\partial h^{\alpha}_{i,rs}}\delta^{\alpha\theta}_{\gamma\omega}\eta_{\theta\beta}h^{\beta}_{i,s}=0\,, \tag{2.2b}$$

and

$$\frac{\partial A}{\partial h^{\alpha}_{i}}\delta^{\alpha\theta}_{\gamma\omega}\eta_{\theta\beta}h^{\beta}_{i}+\frac{\partial A}{\partial h^{\alpha}_{i,r}}\delta^{\alpha\theta}_{\gamma\omega}\eta_{\theta\beta}h^{\beta}_{i,r}+\frac{\partial A}{\partial h^{\alpha}_{i,rs}}\delta^{\alpha\theta}_{\gamma\omega}\eta_{\theta\beta}h^{\beta}_{i,rs}=0\,, \tag{2.2c}$$

respectively, where $\delta^{\alpha\theta}_{\gamma\omega}$ is the generalized Kronecker delta

$$\delta^{\alpha\theta}_{\gamma\omega}=\delta^{\alpha}_{\gamma}\delta^{\theta}_{\omega}-\delta^{\alpha}_{\omega}\delta^{\theta}_{\gamma}\,.$$

Details of these calculations can be found in Ref. 5, Sec. 4. Here we have made use of the relation

$$\left.\frac{\partial\mathcal{L}^{\alpha}_{\beta}}{\partial u^{\gamma\omega}}\right|_{u^{\mu\nu}=0}=-\frac{1}{2}\delta^{\alpha\theta}_{\gamma\omega}\eta_{\theta\beta}\,.$$

To use the invariance identities (2.2) we expand them as

$$\frac{\partial A}{\partial h^{\gamma}_{j,rs}}=\frac{\partial A}{\partial h^{\omega}_{i,rs}}\eta^{\omega\alpha}h^{j}_{\alpha}\eta_{\gamma\beta}h^{\beta}_{i}\,, \tag{2.3a}$$

$$\frac{\partial A}{\partial h^{\gamma}_{j,r}}=\frac{\partial A}{\partial h^{\omega}_{i,r}}\eta^{\omega\alpha}h^{j}_{\alpha}\eta_{\gamma\beta}h^{\beta}_{i}-\frac{2\partial A}{\partial h^{\gamma}_{i,rs}}h^{j}_{\alpha}h^{\alpha}_{i,s}+\frac{2\,\partial A}{\partial h^{\omega}_{i,rs}}\eta^{\omega\alpha}h^{j}_{\alpha}\eta_{\gamma\beta}h^{\beta}_{i,s}\,, \tag{2.3b}$$

and

$$\begin{aligned}\frac{\partial A}{\partial h^{\gamma}_{j}}=&\frac{\partial A}{\partial h^{\omega}_{i}}\eta^{\omega\alpha}h^{j}_{\alpha}\eta_{\gamma\beta}h^{\beta}_{i}-\frac{\partial A}{\partial h^{\gamma}_{i,r}}h^{j}_{\alpha}h^{\alpha}_{i,r}\\&+\frac{\partial A}{\partial h^{\omega}_{i,r}}\eta^{\omega\alpha}h^{j}_{\alpha}\eta_{\gamma\beta}h^{\beta}_{i,r}-\frac{\partial A}{\partial h^{\gamma}_{i,rs}}h^{j}_{\alpha}h^{\alpha}_{i,rs}\\&+\frac{\partial A}{\partial h^{\omega}_{i,rs}}\eta^{\omega\alpha}h^{j}_{\alpha}\eta_{\gamma\beta}h^{\beta}_{i,rs}\,,\end{aligned} \tag{2.3c}$$

respectively, where h^{j}_{α} is the inverse of h^{α}_{j}.

The proof of the result is patterned after that of Noriega and Schifini[9] and amounts to showing that the differential dA, which is by definition linear in dh^{α}_{i}, $dh^{\alpha}_{i,j}$, and $dh^{\alpha}_{i,jk}$, can be expressed in terms that are linear in just dg_{ij}, $dg_{ij,k}$, and $dg_{ij,kh}$. From (1.1) it is possible to obtain the relations between dg_{ij} and dh^{α}_{i}, etc., by taking the appropriate derivatives and differentials. These relations can be expressed as

$$dh^{\omega}_{i}=\eta^{\gamma\omega}h^{j}_{\gamma}\,dg_{ij}-\eta^{\gamma\omega}h^{j}_{\gamma}h^{\alpha}_{i}\eta_{\alpha\beta}\,dh^{\beta}_{j}\,, \tag{2.4a}$$

$$\begin{aligned}dh^{\omega}_{i,k}=&\eta^{\gamma\omega}h^{j}_{\gamma}\,dg_{ij,k}-\eta^{\gamma\omega}h^{j}_{\gamma}h^{\alpha}_{i}\eta_{\alpha\beta}\,dh^{\beta}_{j,k}\\&-\eta^{\gamma\omega}h^{j}_{\gamma}h^{\alpha}_{i,k}\eta_{\alpha\beta}\,dh^{\beta}_{j}-\eta^{\gamma\omega}h^{j}_{\gamma}h^{\beta}_{j,k}\eta_{\alpha\beta}\,dh^{\alpha}_{i}\,,\end{aligned} \tag{2.4b}$$

and

$$\begin{aligned}dh^{\omega}_{i,kh}=&\eta^{\gamma\omega}h^{j}_{\gamma}\,dg_{ij,kh}-\eta^{\gamma\omega}h^{j}_{\gamma}h^{\alpha}_{i}\eta_{\alpha\beta}\,dh^{\beta}_{j,kh}\\&-\eta^{\gamma\omega}h^{j}_{\gamma}h^{\beta}_{j,h}\eta_{\alpha\beta}\,dh^{\alpha}_{i,k}-\eta^{\gamma\omega}h^{j}_{\gamma}h^{\alpha}_{i,k}\eta_{\alpha\beta}\,dh^{\beta}_{j,h}\\&-\eta^{\gamma\omega}h^{j}_{\gamma}h^{\beta}_{j,k}\eta_{\alpha\beta}\,dh^{\alpha}_{i,h}-\eta^{\gamma\omega}h^{j}_{\gamma}h^{\alpha}_{i,h}\eta_{\alpha\beta}\,dh^{\beta}_{j,k}\\&-\eta^{\gamma\omega}h^{j}_{\gamma}h^{\alpha}_{i,kh}\eta_{\alpha\beta}\,dh^{\beta}_{j}-\eta^{\gamma\omega}h^{j}_{\gamma}h^{\beta}_{j,kh}\eta_{\alpha\beta}\,dh^{\alpha}_{i}\,.\end{aligned} \tag{2.4c}$$

We begin by substituting (2.3) and (2.4) into twice the differential dA, i.e.,

$$\begin{aligned}2\,dA=&\frac{\partial A}{\partial h^{\omega}_{i}}dh^{\omega}_{i}+\frac{\partial A}{\partial h^{\omega}_{i,k}}dh^{\omega}_{i,k}+\frac{\partial A}{\partial h^{\omega}_{i,kh}}dh^{\omega}_{i,kh}\\&+\frac{\partial A}{\partial h^{\gamma}_{j}}dh^{\gamma}_{j}+\frac{\partial A}{\partial h^{\gamma}_{j,r}}dh^{\gamma}_{j,r}+\frac{\partial A}{\partial h^{\gamma}_{j,rs}}dh^{\gamma}_{j,rs}\end{aligned}$$

to obtain (upon cancellation of like terms)

$$\begin{aligned}2\,dA=&\frac{\partial A}{\partial h^{\omega}_{i}}\eta^{\gamma\omega}h^{j}_{\gamma}\,dg_{ij}+\frac{\partial A}{\partial h^{\omega}_{i,k}}\eta^{\gamma\omega}h^{j}_{\gamma}\,dg_{ij,k}-\frac{\partial A}{\partial h^{\omega}_{i,k}}\eta^{\gamma\omega}h^{j}_{\gamma}h^{\beta}_{j,k}\eta_{\alpha\beta}\,dh^{\alpha}_{i}+\frac{\partial A}{\partial h^{\omega}_{i,kh}}\eta^{\gamma\omega}h^{j}_{\gamma}\,dg_{ij,kh}\\&-\frac{2\,\partial A}{\partial h^{\omega}_{i,kh}}\eta^{\gamma\omega}h^{j}_{\gamma}h^{\beta}_{j,h}\eta_{\alpha\beta}\,dh^{\alpha}_{i,k}-\frac{\partial A}{\partial h^{\omega}_{i,kh}}\eta^{\gamma\omega}h^{j}_{\gamma}h^{\beta}_{j,kh}\,\eta_{\alpha\beta}\,dh^{\alpha}_{i}\\&-\frac{\partial A}{\partial h^{\gamma}_{i,r}}h^{j}_{\alpha}h^{\alpha}_{i,r}\,dh^{\gamma}_{j}-\frac{\partial A}{\partial h^{\gamma}_{i,rs}}h^{j}_{\alpha}h^{\alpha}_{i,rs}\,dh^{\gamma}_{j}-\frac{2\,\partial A}{\partial h^{\gamma}_{i,rs}}h^{j}_{\alpha}h^{\alpha}_{i,s}\,dh^{\alpha}_{j,r}\,.\end{aligned}$$

By substituting (2.4a) and (2.4b) into the third, fifth, and sixth terms, we find that

$$\begin{aligned}2\,dA=&\frac{\partial A}{\partial h^{\omega}_{i}}\eta^{\gamma\omega}h^{j}_{\gamma}\,dg_{ij}+\frac{\partial A}{\partial h^{\omega}_{i,k}}\eta^{\gamma\omega}h^{j}_{\gamma}\,dg_{ij,k}-\frac{\partial A}{\partial h^{\omega}_{i,k}}\eta^{\gamma\omega}h^{r}_{\gamma}h^{\beta}_{r,k}h^{j}_{\beta}\,dg_{ij}+\frac{\partial A}{\partial h^{\omega}_{i,k}}\eta^{\gamma\omega}h^{r}_{\gamma}h^{\beta}_{r,k}h^{j}_{\beta}h^{\sigma}_{i}\eta_{\sigma\tau}\,dh^{\tau}_{j}\\&+\frac{\partial A}{\partial h^{\omega}_{i,kh}}\eta^{\gamma\omega}h^{j}_{\gamma}\,dg_{ij,kh}-\frac{2\,\partial A}{\partial h^{\omega}_{i,kh}}\eta^{\gamma\omega}h^{r}_{\gamma}h^{\beta}_{r,h}h^{j}_{\beta}\,dg_{ij,k}+\frac{2\,\partial A}{\partial h^{\omega}_{i,kh}}\eta^{\gamma\omega}h^{r}_{\gamma}h^{\beta}_{k,h}h^{j}_{\beta}h^{\sigma}_{i}\eta_{\sigma\tau}\,dh^{\tau}_{j,k}\\&+\frac{2\,\partial A}{\partial h^{\omega}_{i,kh}}\eta^{\gamma\omega}h^{r}_{\gamma}h^{\beta}_{r,h}h^{j}_{\beta}h^{\sigma}_{i,k}\eta_{\sigma\tau}\,dh^{\tau}_{j}+\frac{2\,\partial A}{\partial h^{\omega}_{i,kh}}\eta^{\gamma\omega}h^{r}_{\gamma}h^{\beta}_{r,h}h^{j}_{\beta}h^{\sigma}_{j,k}\eta_{\sigma\tau}\,dh^{\tau}_{i}-\frac{\partial A}{\partial h^{\omega}_{i,kh}}\eta^{\gamma\omega}h^{r}_{\gamma}h^{\beta}_{r,kh}h^{j}_{\beta}\,dg_{ij}\\&+\frac{\partial A}{\partial h^{\omega}_{i,kh}}\eta^{\gamma\omega}h^{r}_{\gamma}h^{\beta}_{r,kh}h^{j}_{\beta}h^{\sigma}_{i}\eta_{\sigma\tau}\,dh^{\tau}_{j}-\frac{\partial A}{\partial h^{\gamma}_{i,r}}h^{j}_{\alpha}h^{\alpha}_{i,r}\,dh^{\gamma}_{j}-\frac{\partial A}{\partial h^{\gamma}_{i,rs}}h^{j}_{\alpha}h^{\alpha}_{i,rs}\,dh^{\gamma}_{j}-\frac{2\,\partial A}{\partial h^{\gamma}_{i,rs}}h^{j}_{\alpha}\,h^{\alpha}_{i,s}\,dh^{\gamma}_{j,r}\,.\end{aligned}$$

The seventh and fourteenth terms cancel by means of (2.3a), as do the eleventh and thirteenth. Application of (2.3b) to the fourth, eighth, and twelfth terms and (2.4a) to the ninth term leads to

$$2\,dA = \frac{\partial A}{\partial h^{\omega}_{i}}\eta^{\gamma\omega}h^{j}_{\gamma}\,dg_{ij} + \frac{\partial A}{\partial h^{\omega}_{i,k}}\eta^{\gamma\omega}h^{j}_{\gamma}\,dg_{ij,k} - \frac{\partial A}{\partial h^{\omega}_{i,k}}\eta^{\gamma\omega}h^{r}_{\gamma}h^{\beta}_{r,k}h^{j}_{\beta}\,dg_{ij} + \frac{2\,\partial A}{\partial h^{\tau}_{i,kh}}h^{r}_{\alpha}h^{\alpha}_{i,k}h^{\beta}_{r,h}h^{j}_{\beta}\,dh^{\tau}_{j}$$
$$+ \frac{\partial A}{\partial h^{\omega}_{i,kh}}\eta^{\gamma\omega}h^{j}_{\gamma}\,dg_{ij,kh} - \frac{2\,\partial A}{\partial h^{\omega}_{i,kh}}\eta^{\gamma\omega}h^{r}_{\gamma}h^{\beta}_{r,h}h^{j}_{\beta}\,dg_{ij,k} + \frac{2\,\partial A}{\partial h^{\omega}_{i,kh}}\eta^{\gamma\omega}h^{r}_{\gamma}h^{\beta}_{r,h}h^{s}_{\beta}h^{\sigma}_{s,k}h^{j}_{\sigma}\,dg_{ij}$$
$$- \frac{2\,\partial A}{\partial h^{\omega}_{i,kh}}\eta^{\gamma\omega}h^{r}_{\gamma}h^{\beta}_{r,h}h^{j}_{\beta}h^{\sigma}_{j,k}h^{s}_{\sigma}h^{\tau}_{i}\eta_{\tau\alpha}\,dh^{\alpha}_{s} - \frac{\partial A}{\partial h^{\omega}_{i,kh}}\eta^{\gamma\omega}h^{r}_{\gamma}h^{\beta}_{r,kh}h^{j}_{\beta}\,dg_{ij}\,.$$

The fourth and eighth terms cancel by (2.3a) and, upon regrouping terms, we have the desired result, viz.,

$$2\,dA = \left(\frac{\partial A}{\partial h^{\omega}_{i}}\eta^{\gamma\omega}h^{j}_{\gamma} - \frac{\partial A}{\partial h^{\omega}_{i,k}}\eta^{\gamma\omega}h^{r}_{\gamma}h^{\beta}_{r,k}h^{j}_{\beta} + \frac{2\,\partial A}{\partial h^{\omega}_{i,kh}}\eta^{\gamma\omega}h^{r}_{\gamma}h^{\beta}_{r,h}h^{s}_{\beta}h^{\sigma}_{s,k}h^{j}_{\sigma} - \frac{\partial A}{\partial h^{\omega}_{i,kh}}\eta^{\gamma\omega}h^{r}_{\gamma}h^{\beta}_{r,kh}\,h^{j}_{\beta}\right)dg_{ij}$$
$$+ \left(\frac{\partial A}{\partial h^{\omega}_{i,k}}\eta^{\gamma\omega}\,h^{j}_{\gamma} - \frac{2\,\partial A}{\partial h^{\omega}_{i,kh}}\eta^{\gamma\omega}h^{r}_{\gamma}h^{\beta}_{r,h}h^{j}_{\beta}\right)dg_{ij,k} + \frac{\partial A}{\partial h^{\omega}_{i,kh}}\eta^{\gamma\omega}h^{j}_{\gamma}\,dg_{ij,kh}\,.$$

Thus we have proved the following lemma.

Lemma: If a quantity A is a concomitant of the frame field and its first two derivatives, i.e.,

$$A = A(h^{\alpha}_{i};h^{\alpha}_{i,j};h^{\alpha}_{i,jk})\,,$$

which is invariant under the connected component of the identity of the signature group, then A is a concomitant of the metric and its first two derivatives, i.e.,

$$A = A(g_{ij};g_{ij,k};g_{ij,kh})\,.$$

We immediately have the following corollary.

Corollary: The derivatives of A with respect to g_{ij} and its derivatives can be expressed in terms of the derivatives of A with respect to h^{α}_{i} and its derivatives as

$$\frac{\partial A}{\partial g_{ij}} = \frac{1}{2}\left(\frac{\partial A}{\partial h^{\omega}_{i}}\eta^{\gamma\omega}h^{j}_{\gamma} - \frac{\partial A}{\partial h^{\omega}_{i,k}}\eta^{\gamma\omega}h^{r}_{\gamma}h^{\beta}_{r,k}h^{j}_{\beta}\right.$$
$$+ \frac{2\,\partial A}{\partial h^{\omega}_{i,kh}}\eta^{\gamma\omega}h^{r}_{\gamma}h^{\beta}_{r,h}h^{s}_{\beta}h^{\sigma}_{s,k}h^{j}_{\sigma}$$
$$\left. - \frac{\partial A}{\partial h^{\omega}_{i,kh}}\eta^{\gamma\omega}h^{r}_{\gamma}h^{\beta}_{r,kh}h^{j}_{\beta}\right),$$

$$\frac{\partial A}{\partial g_{ij,k}} = \frac{1}{2}\frac{\partial A}{\partial h^{\omega}_{i,k}}\eta^{\gamma\omega}h^{j}_{\gamma} - \frac{\partial A}{\partial h^{\omega}_{i,kh}}\eta^{\gamma\omega}h^{r}_{\gamma}h^{\beta}_{r,h}h^{j}_{\beta}\,,$$

and

$$\frac{\partial A}{\partial g_{ij,kh}} = \frac{1}{2}\frac{\partial A}{\partial h^{\omega}_{i,kh}}\eta^{\gamma\omega}h^{j}_{\gamma}\,.$$

At first glance the right-hand sides do not appear to be symmetric in i and j, however, this can be established using the invariance identities (2.3).

It is also possible to establish the following corollary.

Corollary: The two Euler–Lagrange expressions for A, viz.,

$$\mathscr{E}^{i}_{\alpha} \equiv \frac{\partial A}{\partial h^{\alpha}_{i}} - \frac{\partial}{\partial x^{j}}\left(\frac{\partial A}{\partial h^{\alpha}_{i,j}}\right) + \frac{\partial^{2}}{\partial x^{k}\,\partial x^{j}}\left(\frac{\partial A}{\partial h^{\alpha}_{i,jk}}\right)$$

and

$$E^{ij} \equiv \frac{\partial A}{\partial g_{ij}} - \frac{\partial}{\partial x^{k}}\left(\frac{\partial A}{\partial g_{ij,k}}\right) + \frac{\partial^{2}}{\partial x^{h}\,\partial x^{k}}\left(\frac{\partial A}{\partial g_{ij,kh}}\right),$$

are related by

$$E^{ij} = \tfrac{1}{2}\mathscr{E}^{i}_{\alpha}\eta^{\alpha\beta}h^{j}_{\beta}$$

or, equivalently,

$$\mathscr{E}^{i}_{\alpha} = 2E^{ij}h^{\beta}_{j}\eta_{\beta\alpha}\,.$$

Thus if one Euler–Lagrange expression vanishes, so does the other.

By virtue of the above lemma and its corollaries we have just established the following theorem.

Theorem: Concomitants of the following three types are equivalent:

(i) $A = A(g_{ij};g_{ij,k};g_{ij,kh})$;

(ii) $A = A(h^{\alpha}_{i};h^{\alpha}_{i,j};h^{\alpha}_{i,jk})$

and A is invariant under a signature group transformation; and, if $n = 4$,

(iii) $A = A(\sigma_{iAX'};\sigma_{iAX',j};\sigma_{iAX',jk})$

and A is invariant under a spin transformation.

Corollary: If a Lagrangian is one of the above types then the Euler–Lagrange equations obtained by varying g_{ij}, h^{α}_{i}, or $\sigma_{iAX'}$ yield the same results.

We shall now give two examples of the usefulness of these results.

III. DISCUSSION

Lovelock[10] showed that the most general tensor

$$A^{rs} = A^{rs}(g_{ij};g_{ij,k};g_{ij,kh})$$

in a four-dimensional space that satisfies

$$A^{rs}{}_{|s} \equiv 0 \tag{3.1}$$

is

$$A^{rs} = aG^{rs} + bg^{rs}\,, \tag{3.2}$$

where a and b are constants and G^{rs} is the Einstein tensor. By using the result of the previous section we immediately obtain the corresponding theorem of Anderson and Lovelock,[7] viz., if

$$A^{rs} = A^{rs}(\sigma_{iAX'};\sigma_{iAX',j};\sigma_{iAX',jk})$$

is a spin-tensor in a four-dimensional space which is invariant under arbitrary spin transformations and satisfies (3.1), then A^{rs} is given by (3.2).

Some authors[11] have suggested that the electromagnetic tensor might be built out of the frame field and its derivatives, i.e.,

$$F_{rs} = F_{rs}(h^{\alpha}_{i};h^{\alpha}_{i,j};h^{\alpha}_{i,jk}) , \quad F_{sr} = -F_{rs} ,$$

and

$$F_{rs|t} + F_{tr|s} + F_{st|r} \equiv 0 .$$

An equivalent problem is to consider the dual of F_{rs}, i.e.,

$$^{*}F^{rs} = \epsilon^{rstu} F_{tu} ,$$

where ϵ^{rstu} is the four-dimensional Levi-Civita symbol, with

$$^{*}F^{rs} = {}^{*}F^{rs}(h^{\alpha}_{i};h^{\alpha}_{i,j};h^{\alpha}_{i,jk}) , \quad {}^{*}F^{sr} = -{}^{*}F^{rs} ,$$

and

$$^{*}F^{rs}{}_{|s} \equiv 0 .$$

If we demand that $^{*}F^{rs}$ (or F_{rs}) be invariant under a frame field rotation then our result, coupled with that of Lovelock,[10] implies that there are no such tensors since A^{rs} as given by (3.2) is symmetric.

It is clear that we must study what effect the introduction of additional fields will have.

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Local linearization stability

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It is shown that Einstein's equations are always linearization stable around any finite region of space-time. Let (Ω, g^0_{ab}) be any region of space-time, admitting a compact Cauchy surface *with nonempty smooth boundary*, and with g^0_{ab} a sufficiently smooth solution of the vacuum Einstein equation. It is shown that for any solution g^1_{ab} of the linearized equation and any open region $U \subset \Omega$, there exists a smooth one-parameter family g^λ_{ab} of solutions on U such that $(g^\lambda_{ab}|_{\lambda=0} = g^0_{ab})|_U$ and $((d/d\lambda)g^\lambda_{ab} = g^1_{ab})|_U$. By using a result of Choquet-Bruhat and York [*The Cauchy Problem, General Relativity and Gravitation*, edited by A. Held (Plenum, New York, 1980), Vol. 1] asserting the smoothness of the map that sends initial data into solutions of Einstein's evolution equations the proof of the above theorem is reduced to the proof of a similar theorem for Einstein's constraint equations. The proof of this latter theorem involves the use of the implicit function theorem in Hilbert spaces. This local result on linearization stability asserts, in contrast to the general global case, that linearization about *any* vacuum solution is locally physically meaningful.

I. INTRODUCTION

A substantial fraction of our knowledge about solutions of the equations of general relativity has been obtained by linearizing Einstein's equations about some exact solution. What is the relation between the solution of the linearized equations that we can compute, and the would-be exact solution for which the former is supposed to be an approximation? A full answer to this outstanding question is beyond the scope of our present understanding of the theory. Nevertheless, we can answer a related one that gives us enough confidence in certain linearization results even if it does not give us all the information we would like to obtain: *Given any solution of the linearized equations* ${}^4h_{\mu\nu}$ *about a background metric* ${}^4g_{\mu\nu}$, *does there exist a smooth one-parameter family,* ${}^4g^\lambda_{\mu\nu}$, *of exact solutions such that* ${}^4g^\lambda_{\mu\nu}|_{\lambda=0} = {}^4g^0_{\mu\nu}$ *and* $(d/d\lambda)\,{}^4g^\lambda_{\mu\nu}|_{\lambda=0} = {}^4h_{\mu\nu}$? When the answer is affirmative, then we will say that Einstein's equations are *linearization stable* about the given background. This property not only tells us that we are actually approximating some exact solution, but also (with the help of Taylor's formula applied to suitable function spaces) that we are approximating it well.

Linearization stability of Einstein's equations has already been investigated in two cases: when the background metric describes an isolated system, and when it describes a closed cosmology that can be foliated by compact Cauchy surfaces without boundary. Linearization stability occurs for the first case in general,[1,2] and for the second case provided the background metric does not possess any continuous isometry.[2–6] If it does have isometries there are necessary and sufficient conditions for the directions ${}^4h_{\mu\nu}$ to be stable.

Although the two cases mentioned above include many applications of physical interest, they do not cover all of them. In fact, most of the exact solutions we know today cannot be extended (with physically plausible sources) to asymptotically flat spaces or to closed cosmologies. Such is the case, for example, for all the axisymmetric, stationary, and cylindrically symmetric space-times. On the other hand, the causal character of Einstein's equations assures us that existence of solutions in localized regions can be discussed independent of the asymptotic properties of space-time. Thus a local result on linearization stability is not only desirable but is also natural.

A suitable version of this local result, which we shall prove below, is the following theorem.

Local Linearization Stability Theorem: Let $(\Omega, {}^4g^0_{\mu\nu})$ be a region of space-time that is compact, with smooth boundary, globally hyperbolic, and with ${}^4g^0_{ab} \in H^6(\Omega)$. Then for any solution ${}^4h_{ab} \in H^6(\Omega)$ of the linearized equations and any open region $U \subset \Omega$ there exists a one-parameter family ${}^4g^\lambda_{ab} \in H^5(\Omega)$ of exact solutions on U such that

$$ {}^4g^\lambda_{ab}\,|_{\lambda=0} = {}^4g^0_{ab}\,|_U \quad \text{and} \quad \frac{d}{d\lambda}\,{}^4g^\lambda_{ab}\,|_{\lambda=0} = {}^4h_{ab}\,|_U \,. $$

Here $H^s(\Omega)$ denotes the Sobolev space of functions that are square integrable together with derivatives up to order s (Ref. 7). Note that the existence of the one-parameter family of solutions ${}^4g^\lambda_{ab}$ is only asserted on regions strictly contained in Ω. This is because for $\lambda \neq 0$ the region that is globally hyperbolic with respect to ${}^4g^\lambda_{ab}$ may be strictly contained in Ω. We shall prove local linearization stability for the vacuum Einstein equations only: more generally we could consider the system of Einstein's equations plus those describing the evolution of matter fields. If the latter equations are themselves locally linearization stable and if the whole system is hyperbolic we expect that the proof of the above theorem can be extended to cover the case with sources. (See, however, Ref. 8.)

Our first step in the proof of the above theorem is the usual reduction to a proof of linearization stability for the constraint equations on any Cauchy surface Σ of $(\Omega, {}^4g^0_{ab})$. Our second step is to prove linearization stability for the constraint equations.

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II. REDUCTION OF THE PROBLEM TO LINEARIZATION STABILITY OF THE CONSTRAINT EQUATIONS

Let Σ be any Cauchy hypersurface of the globally hyperbolic space-time $(\Omega, {}^4g^0_{ab})$. On Σ, ${}^4g^0_{ab}$ and ${}^4h_{ab}$ induce initial data sets (g^0_{ab}, π^{ab}_0), and $(h^1_{ab}, \omega^{ab}_1)$, respectively. The first set automatically satisfies the exact constraint equations, the second the linearized ones. Assume there exists a differentiable one-parameter family of solutions of the constraint equations such that

$$({}^4g_{ab}(\lambda), {}^4\pi^{ab}(\lambda))|_{\lambda=0} = (g^0_{ab}, \pi^{ab}_0)$$

and

$$\frac{d}{d\lambda}({}^4g_{ab}(\lambda), {}^4\pi^{ab}(\lambda))\Big|_{\lambda=0} = (h_{ab}, \omega^{ab}) .$$

Then the following theorem asserts that for any open $U \subset \Omega$, there exists a differentiable one-parameter family of solution of the full Einstein equations.

Cauchy Stability for the Einstein Equations[2,9]*:* Let $(\Omega, {}^4g^0_{ab})$ be a globally hyperbolic, compact region of space-time satisfying the vacuum Einstein equations with ${}^4g^0_{ab} \in H^6(\Omega)$. Then for any open $U \subset \Omega$ and any Cauchy surface there exists a neighborhood W of (g^0_{ab}, π^{ab}_0) in $H^5(\Sigma) \times H^5(\Sigma)$ such that the mapping from initial data to solutions of the reduced Einstein equations exists and is differentiable (C^1) from W to a neighborhood of ${}^4g^0_{ab}$ in $H^5(\Omega)$.

Thus the problem reduces to showing that the constraint equations are linearization stable.

III. LINEARIZATION STABILITY OF THE CONSTRAINTS

A. Submersion version

The implicit function theorem in Banach spaces is the proper tool to prove linearization stability: the differential equation is considered an implicit description of its solution; it can be inverted—that is, solved— in a neighborhood of a solution if its linearization satisfies certain conditions. In the convenient "submersion" version these conditions demand essentially that the linearized equations can be solved for an arbitrary source. More precisely we have the *Fischer–Marsden sufficient condition*[2,4]*:* Let X, Y be Banach manifolds and $\phi: X \to Y$ a C^1 map. Let $x_0 \in X$ be a solution, $\phi(x_0) = 0$. Suppose that its differential $D\phi_x: TX \to TY$ is surjective and that its kernel has closed complement in TX. Then the equation $\phi(x) = 0$ is linearization stable at x_0.

In our application we will take X to be the $H^2(\Sigma) \times H^1(\Sigma)$ space of initial data (g_{ab}, π^{ab}) on Σ (Ref. 10) and Y the $H^0(\Sigma) \times H^0(\Sigma)$ space of scalar and vector fields (N, N^a) on Σ. The point x_0 is the unperturbed solution (g^0_{ab}, π^{ab}_0), TX and TY are identified with X and Y, respectively, ϕ is the constraint map,

$$\phi(g,\pi) = (H_0 := R(g) + \pi_{ab}\pi^{ab} - \pi^2, H^a := D_b \pi^{ab}) ,$$

and $D\phi_x$ is the constraint map linearized at (g^0_{ab}, π^{ab}_0). Because of the special form of ϕ we can actually show that it is a C^1 map from $H^2(\Sigma) \times H^1(\Sigma)$ to $H^0(\Sigma)$ (Ref. 11). Since $D\phi_x$ is a continuous linear map, its kernel is closed; but TX is a Hilbert space and so the complement of kernel $D\phi_x$ is also closed. Thus we only have to prove surjectivity.

Suppose the contrary, namely that there is some non-vanishing $(N, N^a) \in Y$ that is not the image of any element of X. Since Y is a Hilbert space we can take (N, N^a) orthogonal to the range of $D\phi_x$ (which is closed),

$$\int_\Sigma (N, N^a) \cdot D\phi_{x_0}(h,\omega) d\Sigma = 0, \quad \text{for all } (h,\omega) \in X.$$

Following Choquet-Bruhat and York[2] we now consider the Hamiltonian for general relativity, $H: X \to \mathbb{R}$,

$$H = \int_\Sigma (NH_0 + N^a H_a) d\Sigma .$$

Its differential evaluated at the solution $x_0 = (g^0, \pi_0)$,

$$DH_{(g^0,\pi_0)}(h,\omega) = \int_\Sigma (NDH_0 + N^a DH_a) \cdot (h,\omega)$$

$$= \int_\Sigma (N, N^a) \cdot D\phi_{x_0}(h,\omega) d\Sigma$$

vanishes for all $(h,\omega) \in X$ by virtue of the orthogonality condition assumed above.

By restricting (h,ω) to be of the form $h_{ab} = \phi g^0_{ab}$, $\omega^{ab} = \sqrt{g} D^{(a} l^{b)}$, for arbitrary, smooth (ϕ, l^a) that vanish on the boundary, we can see that (N, N^a) is a weak solution of an elliptic system of equations. The coefficients of this system (g^{ab}_0, π^0_{ab} and their derivatives) are in such Sobolev spaces that one can show (N, N^a) is actually in $H^2(\Sigma) \times H^2(\Sigma)$ (Ref. 12).

Integrating by parts and using Hamilton's equation for general relativity,[13] we get

$$DH_{(g^0,\pi_0)}(h,\omega) = \int_\Sigma (- \dot{\pi}^{ab} h_{ab} + \dot{g}_{ab} \omega^{ab}) d\Sigma$$

$$- \int_{\partial\Sigma} F^l dS_l = 0 \quad \forall (h,\omega) \in X .$$

Here $(\cdot)$ denotes the Lie derivative with respect to the four-vector $Nn^a + N^a$, n^a being the unit normal to Σ. Here F^l are boundary terms arising from partial integration,

$$F^l = - (\tfrac{1}{2} g^{ab} g^{cl} - g^{ac} g^{bl}) (ND_c h_{ab} - h_{ab} D_c N)$$

$$+ 2X_a \omega^{al} + 2(N^a \pi^{bl} - N^l \pi^{ab}) h_{ab} .$$

We first restrict (h,ω) to vanish at the boundary, so that $F^l = 0$, and we then have $(\dot{g}, \dot{\pi}) = 0$. Thus (g,π) must be initial data for a space-time possessing a Killing vector field, namely $Nn^a + N^a$. Next we allow ω^{ab} to take arbitrary values also at the boundary and we find

$$0 = \int_{\partial\Sigma} F^l dS_l = 2 \int_{\partial\Sigma} N_a \omega^{al} dS_l ,$$

hence $N^a|_{\partial\Sigma} = 0$. Similarly, by letting h_{ab} and $D_l h_{ab}$ be arbitrary on $\partial\Sigma$ we conclude $N|_{\partial\Sigma} = D_a N|_{\partial\Sigma} = 0$. But there is no Killing vector field with these boundary properties.[14] Thus we here arrived at a contradiction and so we conclude $D\phi_x$ is a surjective map. This completes the proof of linearization stability.

B. York decomposition version

Here we construct, for any linearized solution, a particular one-parameter family of exact solutions. This also constitutes an alternative proof of linearization stability. We as-

sume that the initial data for the background solution satisfy $\pi_0 = 0$—that is, the background space-time admits a maximal slice. This condition is not very restrictive since the existence of maximal slices for space-time regions of the type we are using here has been established.[15] (We note that in the submersion version this condition was not needed.)

Let the solution be of the form[16]

$$g_{ab}(\lambda) = \hat{g}_{ab}(\lambda)\phi^4(\lambda),$$
$$\pi^{ab}(\lambda) = \rho^{-6}(\pi^{ab}(\lambda) + \lambda^2\Psi^{ab}),$$

with

$$\hat{g}_{ab}(\lambda) := g^0_{ab} + \lambda h_{ab},$$
$$\hat{\pi}^{ab}(\lambda) := \pi^{ab}_0 + \lambda\omega^{ab},$$
$$\phi(\lambda) := (1 + \lambda^2\chi),$$
$$\Psi^{ab}(\lambda) := 2(\hat{D}^{(a}l^{b)} - \tfrac{1}{3}\hat{g}^{ab}\hat{D}_c l^c)\sqrt{\hat{g}},$$

where (g^0_{ab}, π^{ab}_0) is the background solution, (h_{ab}, ω^{ab}) the linearized one, and D_a is the covariant derivative associated with the conformal metric $\hat{g}_{ab}(\lambda)$. The functions ϕ and l^a are to be determined by solving the constraint equations with the boundary conditions

$$\phi|_{\partial\Sigma} = 1, \quad l^b|_{\partial\Sigma} = 0.$$

To show existence of such solutions $(\chi(\lambda), l^b(\lambda)) \in H^2_0(\Sigma) \times H^1_0(\Sigma)$ that are smooth functions of λ we use the implicit function theorem on Banach spaces. We consider the constraint equations as an implicit relation between the variables χ, l^b, and λ:

$$\lambda^2 f(\chi, l^b, \lambda) := \lambda^2\hat{\Delta}_\lambda\chi - \tfrac{1}{8}(\hat{R}_\lambda\phi - M_\lambda(l^b)\phi^{-7}) + N_\lambda\phi^{-7} = 0,$$
$$\lambda^2 f^b(\chi, l^c, \lambda) := \lambda^2\hat{D}_a\psi^{ab} + \hat{D}_a\hat{\pi}^{ab} + 4\phi^{-1}\pi\hat{D}^b\phi = 0,$$

where $\hat{R}_\lambda$ is the scalar curvature of $\hat{g}_{ab}(\lambda)$, $\Delta_\lambda := \hat{g}^{ab}\hat{D}_a\hat{D}_b$, $M_\lambda = (\hat{\pi}^{ab} + \lambda^2\psi^{ab})(\hat{\pi}^{cd} + \lambda^2\psi^{cd})\hat{g}_{ac}\hat{g}_{bd}$, and $N_\lambda = \hat{\pi}^2_\lambda$.

The pair (f, f^b) is a C^1 function of the three variables into $H^0(\Sigma)$, and $(f, f^b)(0,0,0) = 0$. To apply the implicit function theorem we evaluate the differential of (f, f^b) at $(\chi, l^b) = 0 = \lambda$, holding λ fixed, as a linear map on $(\delta\chi, \delta l^a) \in H^2_0(\Sigma) \times H^1_0(\Sigma)$:

$$Df(0)\cdot(\delta\chi\delta l^a) = \Delta_0\delta\chi - M_0\delta\chi + \tfrac{1}{4}\pi^{ab}_0 D(a^{\delta l}b), \quad (1)$$
$$Df^b(0)\cdot(\delta\chi\delta l^a) = D_a(D^{(a}\delta l^{b)} - \tfrac{1}{3}g^{0ab}D_c\delta l^c). \quad (2)$$

This is a second-order elliptic map on a compact manifold with boundary and with coefficients in Sobolev spaces of high enough order so that if it is injective then it is also surjective,[17] and therefore an isomorphism.

Assume, by contradiction, that the above map is not injective. Then there exists some nonvanishing pair $(\delta\chi, \delta l^b) \in H^2_0(\Sigma) \times H^1_0(\Sigma)$ that is mapped to zero. Contract (2) with δl_b and integrate to obtain

$$\int_\Sigma \delta l_b Df^b(0)\cdot(\delta\chi\delta l^a)d\Sigma = \int_\Sigma \left(D^{(a}\delta l^{b)}\frac{1}{3}g^{0ab}D_c\delta l^c\right)^2 d\Sigma = 0.$$

This implies that δl^b is a conformal Killing vector field in (Σ, g^0_{ab}). It is easy to show by an argument similar to the one in Ref. 12 that there is no conformal Killing vector which can vanish on $\partial\Sigma$, so that $\delta l^b = 0$. Now multiply (1) by $\delta\chi$ and integrate

$$\int_\Sigma \delta\chi Df(0)\cdot(\delta\chi, 0)d\Sigma = -\int_\Sigma \{(D\delta\chi)^2 + M_0(\delta\chi)^2\}d\Sigma = 0.$$

This implies, since $M_0 > 0$ and $\delta\chi|_{\partial\Sigma} = 0$, that $\delta\chi$ also must vanish everywhere. From this contradiction we conclude that (Df, Df^a) is an isomorphism. The implicit function theorem then shows the existence of functions χ and l^b that are smooth in λ. Thus we have shown the existence of the one-parameter family of exact solutions and established linearization stability.

IV. CONCLUSIONS

We have shown in two ways that the source-free Einstein equations, restricted to a local space-time neighborhood, are linearization stable. The first version of the proof shows that the space of solutions is a C^1 manifold in the function-space neighborhood of any particular solution. The second version identifies the free data and constructs the particular family of exact solutions that coincides (for all λ) with the linearized solution on the boundary of the neighborhood.

ACKNOWLEDGMENT

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[2] Y. Choquet-Bruhat and J. W. York, Jr., *The Cauchy Problem, General Relativity and Gravitation*, edited by A. Held (Plenum, New York, 1980).

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[4] A. Fischer and J. Marsden, "Linearization stability of the Einstein equations," Bull. Am. Math. Soc. **79**, 995 (1973).

[5] V. Moncrief, J. Math. Phys. **16**, 493 (1975); **17**, 1893 (1976).

[6] D. Brill and S. Deser, Commun. Math. Phys. **32**, 291 (1973).

[7] For example, the H^0 norm is just the L^2 norm and the $H^1(\Sigma)$ norm given by $\|f\|^2_1 = \int_\Sigma \{f^2 + g^{ab}\nabla_a f\nabla_b f\}d\Sigma$. Here g^{ab} is some Riemannian metric and since Σ is compact the resulting function space does not depend on g^{ab}. We will also use spaces of functions that vanish on the boundary, denoted by $H^s_0(\Sigma)$, which are the completion of $C^\infty_0(\Sigma)$, under the $H^s(\Sigma)$ norm. Thus, for example, if a function $f \in H^1_0(\Sigma)$, then it vanishes (in the L^2 sense) on $\partial\Sigma$.

[8] D. Brill and C. V. Vishveshwara, J. Math. Phys. **27**, 1813 (1986).

[9] T. Kato, Arch. Rat. Mech. Anal. **58**, 181 (1975).

[10] Actually X is the Banach manifold obtained by removing from the Banach space $H^2(\Sigma) \times H^1(\Sigma)$ the points where g_{ab} is not invertible. Note that the assumptions needed in this section are much weaker than those needed to establish Cauchy stability.

[11] As an example we show that R, the scalar curvature, is C^1 as a map from $H^2(\Sigma)$ to $H^0(\Sigma)$. First we prove that R is differentiable, namely that there exists a linear functional $(DR)_g$ from $H^2(\Sigma)$ to $H^0(\Sigma)$ such that, for $\|h\|_{H^2}$ small enough, $\|R(g+h) - R(g) - DR_g\cdot h\|_{H^0} < C\|h\|_{H^2}$. Let $DR\cdot h = -g^{ab}D^2h_{ab} + g^{ab}g^{cd}D_aD_ch_{bd} - h^{ab}R_{ab}$ and note that $R_{ab}(g+h) = R_{ab}(g+h) = R_{ab}(g) + 2D_{[a}\omega_{c]}c_b - 2\omega^c_{d[c}\omega^d_{a]b}$, with $\omega^c_{ab} = (g+h)/2\{D_ah_{bc} + D_bh_{ac} - D_eh_{ab}\}$, to show that $R(g+h) - R(g) - DR_g\cdot h$ has only terms of the form $D^S hD^{S-2}hg^{-3}\Sigma \times (g^{-1}h)^n a_n(g)$. The series appears because the expansion of $(g+h)^{-1}$. Because $H^2(\Sigma) \subset C_0(\Sigma)$ we have pointwise control of g. Thus, if g is invertible, then for all h such that $\|h\|_{H^2}$ is small enough, $(g+h)$ is also

invertible and all the series converge. Next we use for example that $L^4(\Sigma)\subset H^1(\Sigma)$ to bound the terms of the form $(Dh)^2$: $\|(Dh)^2\|_{L^2}=\|Dh\|^2_{L^4}\leqslant C\|Dh\|^2_{H^1}\leqslant C\|h\|^2_{H^2}$. Using the same type of inequalities we can also prove that $DR_{(g)}\cdot h$ is both continuous in h and in g (in the first case as a function from H^2 to H^0 and in the second as a linear map, namely in the norm $\sup_{\|h\|_{H^2}=1}\|DR_{(g)}\cdot h\|_{H^0}$).

[12]Here we can use the following Garding type inequality. Let $L(u)\equiv\Sigma a_k D^k u$ be an elliptic system with coefficients $a_k\in H^k(\Sigma)$, $s_k>n/2+\alpha+k-m$, $\alpha>0$, $n=\dim\Sigma$. Then there exists a $C>0$ such that for all $u\in H^m(\Sigma)$ we have $\|u\|_H M\leqslant C\{\|Lu\|_{H^0}+\|u\|_{H^0}\}$. In our case $m=2$ and we can take $s_k=k$ ($\alpha<\frac{1}{2}$). This inequality, plus the usual arguments using sequences of operators $\{L_n\}$, with smooth coefficients, converging to L, tells us that every weak solution $L(u)=0$ is in $H^2(\Sigma)$. The above inequality is a generalization of the one proved in Ref. 19. See also Ref. 17.

[13]One actually computes the adjoint map ${}^*D\phi_x\ (N,X^a)\to(\sigma,\omega)$, and then substitutes for the evolution equation.

[14]Use Killing transport, as defined in R. Geroch, Commun. Math. Phys. **13**, 180 (1969). [A conformal Killing vector ξ_a (i.e., $\nabla_{(a}\xi_{b)}=\phi g_{ab}$) must satisfy $n^a\nabla_a\xi_b=n^a(F_{ab}+\frac{1}{2}\phi g_{ab})$, $n^a\nabla_a\phi=n^a k_a$, $n^a\nabla_a F_{bc}=n^a(R_{bcad}\xi^d+k_{[b}g_{c]a})$, and $n^aD_a k_b=n^a(\xi^d\nabla_d L_{ab}+\phi L_{ab}+2R_{d(a}F_{b)}{}^d)$, where $L_{ab}=R_{ab}-\frac{1}{6}g_{ab}R$, for arbitrary n^a. Letting $n^a=\partial/\partial t$ for some t we obtain a system of ordinary differential equations on t for the variables (ξ_b,ϕ,F_{ab},k_a). Thus the value at one point of these fields defines the field everywhere.] We see that if the Killing data, (ξ^a,F_{cb}) vanish at one point, they vanish everywhere. Using $\xi^a|_{\partial\Sigma}=0$, when $\xi^a:=Nn^a+N^a$, and decomposing $F_{ab}:=\nabla_a\xi_b$ into tangential and normal parts to $\partial\Sigma$ one finds, $\Theta^{ab}F_{bc}=0$ and $\sigma^{ac}\sigma^{bd}F_{ab}=2n^{[c,d]}r^l\nabla_l N0$, where Θ^{ab} is the metric induced in $\partial\Sigma$, $\sigma^{ab}=g^{0ab}-\Theta^{ab}$ and r^l is the unit normal to $\partial\Sigma$ in Σ. Thus we conclude that the Killing data vanish in $\partial\Sigma$ so that ξ^a vanishes everywhere. In the second version a similar argument is needed, this time using conformal Killing transport, to rule out possible conformal Killing vectors in Σ which vanish on $\partial\Sigma$.

[15]R. Bartnik, Commun. Math. Phys. **94**, 155 (1984), Theorem 4.2.

[16]A similar form of solution was used in Ref. 3 to prove a similar result.

[17]If an injective elliptic system has C^∞ coefficients, then it is also surjective.[18] On the other hand, if an elliptic map L is injective but only has coefficients in certain Sobolev spaces, as is the case for the map under consideration, we also have $\|u\|_2\leqslant C\{\|L(u)\|_0+\|u\|_0\}$, for all $u\in H^2(\Sigma)$, where c is independent of u. This inequality is a generalization to fractional order Sobolev spaces of a theorem of Ref. 19. Let $\{L_n\}$ be a sequence of injective maps with C^∞ coefficients that converges to L. Given any $f\in H^0(\Sigma)$ we then have a sequence $\{u_n\}$ such that $L_n(u_n)=f$. Because the above inequality $\{u_n\}$ is bounded in $H^2(\Sigma)$ and so there is a subsequence that converges weakly to some $u\in H^2(\Sigma)$, and $L(u)=f$ weakly, so L is also surjective.

[18]O. A. Ladyzhenskaya and N. N. Ural'tsera, *Linear and Quasilinear Elliptic Equations* (Academic, New York, 1986), p. 107.

[19]Y. Choquet-Bruhat and D. Christodoulou, Acta Math. **146**, 137 (1981).

Shear-free perfect fluids in general relativity. I. Petrov type N Weyl tensor

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Petrov type N, shear-free, perfect fluid solutions of the Einstein field equations are investigated. It is shown that if the fluid pressure p and energy density w are related by a barotropic equation of state $p = p(w)$ satisfying $w + p \neq 0$, and if the Weyl tensor is of Petrov type N then the fluid's volume expansion is zero but the vorticity is necessarily nonzero. The differential equation determining p as a function of w is given. For this class of solutions the fluid's vorticity vector is orthogonal to the acceleration.

I. INTRODUCTION

There are a number of results in the literature that suggest that the following conjecture holds, in general.

Conjecture: Any shear-free perfect fluid in general relativity, with a barotropic equation of state $p = p(w)$ (w is the energy density and p is the fluid pressure) such that $w + p \neq 0$, has either vanishing vorticity or vanishing expansion.

For example, the conjecture is known to hold in (i) all dust space-times (Ellis[1]), (ii) conformally flat space-times,[2] (iii) spatially homogeneous space-times (King and Ellis[3] and White[4]), (iv) shear-free radiation, $p = \frac{1}{3}w$ (Treciokas and Ellis[5]), (v) the case when the fluid vorticity ω_a and acceleration $\dot{u}_a$ are parallel (White and Collins[6]), and (vi) the case when the magnetic part of the Weyl tensor, with respect to the fluid flow, vanishes (Collins[7]).

Shear-free fluids with a barotropic equation of state are of considerable interest in cosmology from both the theoretical and observational point of view (Friedmann–Robertson–Walker models, Gödel solution, etc.). For example, certain observational aspects of shear-free fluids, which are relevent to cosmology, are most readily highlighted when one considers the formulas for recessional motion, relative red shift, and transverse motion of neighboring galaxies.[2,8] It then readily follows, for example, that shear-free fluid solutions would retain the desirable feature of isotropy of local motion but allow the galactic red shift to be anisotropic if $\dot{u}_a \neq 0$. (The relative measure of this anisotropy would be given by the ratio $3|\dot{u}_a|/\theta$, where $\theta \neq 0$ is the volume expansion.) Consequently, there would be a preferred direction, which coincides with that of $\dot{u}_a$, as indicated by the maximum red shift. On the theoretical side, the general validity of the above conjecture, together with the possibility that relativistic kinetic theory requires perfect fluids to be shear-free,[5] would impart a sense of uniqueness[9] to the Friedmann–Robertson–Walker cosmological models since it has been shown that they are the only physically reasonable space-times which represent an expanding, shear-free, irrotational perfect fluid, on a global scale.

Finally, it is interesting to note that there are Newtonian self-gravitating, shear-free fluids that are expanding and rotating.[2] Therefore, if the conjecture were to be generally valid, then it would be a result that would highlight certain essential differences between fluid dynamics in Newtonian theory and in general relativity. (For an interesting and comprehensive review of shear-free perfect fluids and their applications to cosmology, see Collins.[8])

In this paper, we will be investigating the validity of the above conjecture for Petrov type N space-times. We shall show that any shear-free, perfect fluid source, of a type N space-time in general relativity, where $p = p(w)$ and $w + p \neq 0$, must necessarily be rotating,[10] $\omega \neq 0$, with zero volume expansion, $\theta = 0$. In addition, the differential equation determining p as a function of w will be given. Finally, we will show that for this class of solutions the fluid vorticity vector is orthogonal to the acceleration.

The plan of this article is as follows: Section II contains the main results which are summarized in the statement of the Theorem and its corollary. The proofs are given in Sec. III, and Sec. IV contains some concluding remarks. This paper presupposes a knowledge of the Newman–Penrose[11] formalism (abbreviated NP). All considerations will be local. We have chosen geometrized units so that $8\pi G = 1$, $c = 1$, where G is the Newtonian gravitational constant and c is the speed of light in vacuo. Our conventions for the Riemann and Ricci tensors and the signature of the space-time are those of NP.

II. THE MAIN RESULTS

In this article, we shall be investigating Petrov type N, perfect fluid solutions of Einstein's field equations,

$$R_{ab} - \tfrac{1}{2}Rg_{ab} + Kg_{ab} = -T_{ab}, \tag{2.1}$$

where

$$T_{ab} = (w + p)u_a u_b - pg_{ab}, \quad u_a u^a = 1, \tag{2.2}$$

in which the fluid congruence is shear-free and the pressure satisfies a barotropic equation of state,

$$p = p(w). \tag{2.3}$$

Our main result is the following.

Theorem: For any Petrov type N, shear-free, perfect fluid solution of Einstein's field equations, in which the perfect fluid satisfies a barotropic equation of state $p = p(w)$ such that $w + p \neq 0$, the volume expansion is zero but the vorticity is necessarily nonzero.

We therefore conclude that the conjecture holds for Petrov type N space-times. It then follows that the equation of

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state satisfies a second order, nonlinear differential equation, given in the following.

Corollary: For any Petrov type N, shear-free, perfect fluid solution of Einstein's field equations in which the perfect fluid satisfies a barotropic equation of state $p=p(w)$, with $w+p\neq 0$, the pressure $p(w)$ must be a solution of the differential equation

$$9(w+p)(w+3p-2K)\ddot{p} = (1+3\dot{p})(9\dot{p}w+18\dot{p}K-9\dot{p}p-w-3p+2K), \quad \dot{p}\neq \text{const},$$

with no additional constraints on $p(w)$.

III. PROOF OF THE RESULTS

Let C_{abcd} and u_a denote the Weyl tensor and four-velocity of the fluid, respectively. The assumption that C_{abcd} is of Petrov type N seems to naturally lead to the following specialization of the principal null tetrad $\{l,n,m,\bar{m}\}$. First, l is chosen to be the repeated principal null direction of the Weyl tensor, so that

$$C_{abcd}l^d=0, \tag{3.1}$$

and the NP Weyl tensor components satisfy

$$\Psi_0=\Psi_1=\Psi_2=\Psi_3=0, \quad \Psi_4\neq 0. \tag{3.2}$$

Next, by a null rotation which leaves l fixed, it is possible to make n lie in the two-spaces spanned by l and u. Finally, by rescaling l and n it is then possible to achieve

$$u=(1/\sqrt{2})(l+n). \tag{3.3}$$

From Eqs. (2.1)–(2.3) and (3.3), it follows that the NP components of the trace-free Ricci tensor $S_{ab}\equiv R_{ab}-\frac{1}{4}Rg_{ab}$ satisfy

$$\Phi_{01}=\Phi_{12}=\Phi_{02}=0, \tag{3.4}$$

$$\Phi_{00}=\Phi_{22}=2\Phi_{11}=\tfrac{1}{4}(w+p). \tag{3.5}$$

The Ricci scalar $R\equiv 24\Lambda$ is given by

$$R=w-3p+4K. \tag{3.6}$$

It should be noted at this point that the tetrad is still not fixed uniquely. The remaining tetrad freedom is expressed by the rotation

$$\tilde{l}^a=l^a, \quad \tilde{n}^a=n^a, \quad \tilde{m}^a=e^{i\xi}m^a, \tag{3.7}$$

where ξ is a real function.

The shear tensor σ_{ab}, vorticity tensor ω_{ab}, and expansion θ of the fluid four-velocity (3.3) are given by[12]

$$\sigma_{ab}=A_1\{v_av_b-m_{(a}\bar{m}_{b)}\}+A_2v_{(a}m_{b)}+\bar{A}_2v_{(a}\bar{m}_{b)}+A_3m_am_b+\bar{A}_3\bar{m}_a\bar{m}_b, \tag{3.8}$$

where

$$A_1=-\tfrac{1}{3}2^{-1/2}\{\rho+\bar{\rho}-\mu-\bar{\mu}+2(\epsilon+\bar{\epsilon})-2(\gamma+\bar{\gamma})\},$$
$$A_2=-\tfrac{1}{2}\{\bar{\tau}+\pi+2(\alpha+\bar{\beta})-\bar{\kappa}-\nu\},$$
$$A_3=2^{-1/2}(\bar{\sigma}-\lambda),$$
$$v_a=2^{-1/2}(l_a-n_a),$$

and

$$\omega_{ab}=B_1v_{[a}m_{b]}+\bar{B}_1v_{[a}\bar{m}_{b]}+B_2m_{[a}\bar{m}_{b]}, \tag{3.9}$$

where

$$B_1=\tfrac{1}{2}\{\bar{\tau}+\pi-2(\alpha+\bar{\beta})-\bar{\kappa}-\nu\},$$
$$B_2=-2^{-1/2}\{\rho-\bar{\rho}+\mu-\bar{\mu}\},$$

and

$$\theta=2^{-1/2}\{\epsilon+\bar{\epsilon}-\gamma-\bar{\gamma}-\rho-\bar{\rho}+\mu+\bar{\mu}\}. \tag{3.10}$$

Thus it follows from (3.8) that the fluid is shear-free if and only if

$$\rho+\bar{\rho}-\mu-\bar{\mu}+2(\epsilon+\bar{\epsilon})-2(\gamma+\bar{\gamma})=0, \tag{3.11a}$$
$$\tau+\bar{\pi}+2(\bar{\alpha}+\beta)-\kappa-\bar{\nu}=0, \tag{3.11b}$$
$$\sigma-\bar{\lambda}=0. \tag{3.11c}$$

The next step in the proof requires the explicit injection of Eqs. (3.2), (3.4), and (3.5) into the NP form of the Bianchi identities which after some straightforward manipulations reduce to the following equivalent set:

$$\sigma=\bar{\lambda}, \tag{3.12a}$$
$$\tau+\bar{\pi}+2(\bar{\alpha}+\beta)-\kappa-\bar{\nu}=0, \tag{3.12b}$$
$$\rho-\bar{\mu}=\bar{\rho}-\mu, \tag{3.12c}$$
$$2\kappa\Psi_4-(w+p)(\alpha+\bar{\beta})=0, \tag{3.12d}$$
$$D\Psi_4=(\rho-4\epsilon)\Psi_4, \tag{3.12e}$$
$$\delta\Psi_4=(\tau-4\beta+3\kappa)\Psi_4, \tag{3.12f}$$
$$Dw=\tfrac{3}{2}(w+p)(\bar{\rho}-\mu), \tag{3.12g}$$
$$\Delta w=\tfrac{1}{2}(w+p)(2\gamma+2\bar{\gamma}-2\epsilon-2\bar{\epsilon}+\bar{\rho}-\mu), \tag{3.12h}$$
$$\delta w=3(w+p)(\bar{\alpha}+\beta), \tag{3.12i}$$
$$\dot{p}(\bar{\rho}-\mu-\gamma-\bar{\gamma}+\epsilon+\bar{\epsilon})=-(\gamma+\bar{\gamma}+\epsilon+\bar{\epsilon}), \tag{3.12j}$$
$$3\sigma\Psi_4=\tfrac{1}{2}(w+p)(\bar{\rho}-\mu-\gamma-\bar{\gamma}+\epsilon+\bar{\epsilon}), \tag{3.12k}$$
$$(1+3\dot{p})(\bar{\alpha}+\beta)=\kappa-\bar{\pi}. \tag{3.12l}$$

Imposing the shear-free requirement[13] (3.11a) on Eq. (3.12k) and using (3.12a), (3.12c), and (3.12j), leads to

$$\sigma=\lambda=0, \tag{3.13}$$

and

$$\gamma+\bar{\gamma}=-(\epsilon+\bar{\epsilon})=\tfrac{1}{2}(\bar{\rho}-\mu). \tag{3.14}$$

Thus

$$Dw=\Delta w=\tfrac{3}{2}(w+p)(\bar{\rho}-\mu). \tag{3.15}$$

Using certain of the NP equations (4.2), together with (3.12b) and (3.13), yields

$$\delta(\bar{\alpha}+\beta)=(\bar{\alpha}+\beta)(\bar{\alpha}+3\beta-2\bar{\nu}+2\tau)+\bar{\Psi}_4/2, \tag{3.16}$$

and consequently $\bar{\alpha}+\beta\neq 0$, which implies $\kappa\neq 0$. This indicates that the repeated principal null congruence of the Weyl tensor is nongeodesic, and in addition through the use of Eqs. (3.9) and (3.12b), that the fluid is necessarily rotating. These results are consistent with Oleson's[12] Theorems (4.2), (5.1), and (5.3). The operator δ may now be applied to Eq. (3.12l) to yield the important relation

$$2(\bar{\alpha}+\beta)^2\{(1+3\dot{p})(3\dot{p}-1)+9\ddot{p}(w+p)\}+\bar{\Psi}_4(1+3\dot{p})=0, \tag{3.17}$$

where $\langle\langle\,\dot{}\,\rangle\rangle$ denotes differentiation with respect to w, and where use has been made of Eq. (3.12b) and the NP equa-

tions (4.2b) and (4.2g). Applying the $[\delta, D]$ commutator to w yields, after canceling a $w+p$ factor throughout,

$$\delta(\bar{\rho}-\mu)-2D(\bar{\alpha}+\beta)$$
$$=(\bar{\alpha}+\beta-\bar{\pi}+\kappa)(\bar{\rho}-\mu)$$
$$-2(\bar{\alpha}+\beta)(\bar{\rho}+\epsilon-\bar{\epsilon}). \tag{3.18}$$

From NP equations (4.2k) and (4.2m) and Eq. (3.12c), it follows that

$$\delta(\bar{\rho}-\mu)=(\rho+\bar{\mu})(\bar{\alpha}+\beta)+(\tau-\bar{\nu})(\rho-\bar{\rho})$$
$$+(\kappa-\bar{\pi})(\mu-\bar{\mu}). \tag{3.19}$$

Combining Eqs. (3.18) and (3.19) gives

$$2D(\bar{\alpha}+\beta)=(\bar{\alpha}+\beta)(\rho+\bar{\rho}+3\mu-\bar{\mu}+2\epsilon-2\bar{\epsilon})$$
$$+(\bar{\pi}-\kappa)(\bar{\rho}-\mu). \tag{3.20}$$

Also, NP equations (4.2d) and (4.2e) together with Eqs. (3.14) and (3.19) give

$$2D(\bar{\alpha}+\beta)=(\bar{\alpha}+\beta)(2\bar{\rho}-\rho-2\mu+\bar{\mu}-4\bar{\epsilon})$$
$$+(\bar{\pi}-\kappa)(\bar{\rho}+\mu). \tag{3.21}$$

Next, the NP equations (4.2d), (4.2e), (4.2o), (4.2r) together with Eq. (3.14) imply

$$(D+\Delta)(\bar{\alpha}+\beta)=(\bar{\alpha}+\beta)(2\gamma-2\bar{\epsilon}+\bar{\rho}-\mu)$$
$$-\tfrac{1}{2}(\bar{\rho}+\mu)(\kappa+\tau-\bar{\nu}-\bar{\pi}). \tag{3.22}$$

On the other hand, applying the $[\delta, D-\Delta]$ commutator to w and using Eqs. (3.12i) and (3.15) yields

$$(\Delta-D)(\bar{\alpha}+\beta)$$
$$=(\bar{\alpha}+\beta)(\bar{\rho}-3\mu+\gamma-\bar{\gamma}-\epsilon+\bar{\epsilon}). \tag{3.23}$$

Solving Eqs. (3.22) and (3.23) for $D(\bar{\alpha}+\beta)$ gives

$$2D(\bar{\alpha}+\beta)=(\bar{\alpha}+\beta)(\gamma+\bar{\gamma}+2\mu+\epsilon-3\bar{\epsilon})$$
$$-\tfrac{1}{2}(\bar{\rho}+\mu)(\kappa+\tau-\bar{\nu}-\bar{\pi}). \tag{3.24}$$

Comparing Eqs. (3.20), (3.21), and (3.24) yields the conditions

$$\mu(\bar{\alpha}+\beta)=\mu\{2(\bar{\alpha}+\beta)-\bar{\pi}+\kappa\}=0, \tag{3.25}$$

where use has been made of Eqs. (3.12b) and (3.14). Thus we conclude that

$$\mu=0, \tag{3.26}$$

which implies that

$$\rho=\bar{\rho}. \tag{3.27}$$

Next, we shall show that if $\rho\neq 0$, then necessarily a contradiction follows. This will be done by considering three subcases.

Assumption $\rho\neq 0$: Case (1): $1+3\dot{p}\neq 0, \dot{p}\neq 0$. Equations (3.17) and (3.21) imply, respectively,

$$(\alpha+\bar{\beta})^2 G(w)+2\Psi_4=0, \tag{3.28}$$

where

$$G:=4\{3\dot{p}-1+9\ddot{p}(w+p)/(1+3\dot{p})\} \tag{3.29}$$

and

$$2D(\bar{\alpha}+\beta)=-(\bar{\alpha}+\beta)(4\bar{\epsilon}+3\rho\dot{p}). \tag{3.30}$$

Applying the D operator to Eq. (3.28) yields, after canceling an $\bar{\alpha}+\beta$ factor throughout,

$$\dot{G}=2G(1+3\dot{p})/3(w+p). \tag{3.31}$$

The D operator applied to Eq. (3.12d) gives

$$2D\kappa=\kappa(\rho+4\epsilon). \tag{3.32}$$

Solving Eqs. (3.22) and (3.23) for $\Delta(\bar{\alpha}+\beta)$ leads to

$$2\Delta(\bar{\alpha}+\beta)=(\bar{\alpha}+\beta)(4\gamma+2\rho-3\rho\dot{p}), \tag{3.33}$$

so that the Δ operator may now be applied to Eq. (3.28) to yield

$$\Delta\Psi_4=\Psi_4(5\rho-4\gamma). \tag{3.34}$$

It is now possible, by virtue of Eqs. (3.15), (3.33), and (3.34), to apply the Δ operator to Eq. (3.12d) in order to determine $\Delta\kappa$. We find that

$$2\Delta\kappa=\kappa(4\gamma-3\rho). \tag{3.35}$$

The δ operator applied to Eq. (3.28) and subsequent use of (A4) leads to the following algebraic condition, linear in the spin coefficients,

$$\bar{\nu}+\bar{\pi}-2\kappa-4\tau=0. \tag{3.36}$$

It should be noted that Eqs. (3.28)–(3.36) also hold when $\dot{p}=0$. Next, using Eqs. (3.12b) and (3.12l) in conjunction with (3.36), gives

$$\kappa+3\tau=-6\dot{p}(\bar{\alpha}+\beta). \tag{3.37}$$

Applying δ to Eq. (3.37), and noting that $\kappa+3\tau\neq 0\Leftrightarrow\dot{p}(\bar{\alpha}+\beta)\neq 0$, yields

$$2\tau-\kappa=(\bar{\alpha}+\beta)H(w), \tag{3.38}$$

where use has been made of Eq. (3.36), and where

$$H(w):=3\ddot{p}(w+p)/2\dot{p}-G/8. \tag{3.39}$$

We may now solve for κ, τ, $\bar{\nu}$, and $\bar{\pi}$ in terms of $(\bar{\alpha}+\beta)$ and functions of w:

$$\kappa=-(\bar{\alpha}+\beta)(3H+12\dot{p})/5, \tag{3.40a}$$
$$\tau=(\bar{\alpha}+\beta)(H-6\dot{p})/5, \tag{3.40b}$$
$$\bar{\nu}=(\bar{\alpha}+\beta)(H-21\dot{p}+5)/5, \tag{3.40c}$$
$$\bar{\pi}=-(\bar{\alpha}+\beta)(3H+27\dot{p}+5)/5. \tag{3.40d}$$

Finally, the contradiction follows by applying the D and Δ operators to κ, as given in Eq. (3.40a), and then comparing with Eqs. (3.32) and (3.35), respectively. Specifically, Eqs. (3.32) and (3.40a) imply

$$F(3\dot{p}-1)-3\dot{F}(w+p)=0, \tag{3.41}$$

whereas Eqs. (3.35) and (3.40a) imply

$$F(5-3\dot{p})+3\dot{F}(w+p)=0, \tag{3.42}$$

where

$$F:=-(3H+12\dot{p})/5. \tag{3.43}$$

We conclude that $F=0$ which implies $\kappa=0$, which is impossible.

Case (2)[14]: $\dot{p}=0$. It follows immediately from Eqs. (3.29) and (3.31) that this case is impossible.

Before proceeding to the third and final case of when $1+3\dot{p}=0$, it will prove convenient to use the remaining tetrad freedom (3.7) to make

$$\bar{\alpha}+\beta=\alpha+\bar{\beta}. \tag{A6}$$

It then follows that Ψ_4 and *all* spin coefficients are real in this

chosen tetrad (see the Appendix). All subsequent analysis will be carried out in this tetrad.

Case (3): $1 + 3\dot{p} = 0$. From Eq. (3.12l) we have

$$\kappa = \pi, \tag{3.44}$$

which together with the NP equations (4.2b) and (4.2h) implies

$$\pi(\beta - \alpha) + \Lambda = 0. \tag{3.45}$$

Also, the NP equations (4.2d) and (4.2e) give

$$D(\alpha - \beta) = \rho(\alpha - \beta + \pi),$$

so that the D operator may be applied to Eq. (3.45) ($D\kappa = 0$) to give

$$\kappa^2 = \pi^2 = \tfrac{1}{12}(Q - 2K), \tag{3.46}$$

where Q is a constant of integration determined by

$$w + 3p = Q. \tag{3.47}$$

Since $\kappa = \pi = \text{const}$, then the NP equations (4.2b), (4.2c), and (4.2i) yield

$$\nu - \pi - \alpha + \beta = 0, \tag{3.48}$$

$$D\tau = \rho\tau, \tag{3.49}$$

$$D\nu = \rho\nu, \tag{3.50}$$

while comparison of NP equations (4.2j) and (4.2n) gives

$$2\nu(\alpha - \beta) = 2\nu(\nu - \pi) = \Psi_4 - 2\Phi_{11}. \tag{3.51}$$

Applying the D operator to Eq. (3.51) leads to

$$2\nu^2 = \Psi_4 + 2\Phi_{11} - 3\dot{\Phi}_{11}(w + p), \tag{3.52}$$

which immediately yields

$$2\nu^2 = \Psi_4. \tag{3.53}$$

Substituting Eq. (3.53) into (3.51) gives

$$\Phi_{11} = \nu\pi. \tag{3.54}$$

With the NP equation (4.2n) and Eqs. (3.12f) and (3.44), the δ operator may be applied to Eq. (3.53) to give

$$4\beta = 3(\pi - \tau). \tag{3.55}$$

Equations (3.11b), (3.48), and (3.55) may be combined to yield

$$\pi = 2\tau - \nu. \tag{3.56}$$

Finally, if we now apply the D operator to Eq. (3.56) then it follows that $\rho(2\tau - \nu) = 0$ which implies $2\tau - \nu = 0$ and hence $\kappa = \pi = 0$, which is impossible. Thus we conclude $\rho = 0$ in all cases and the proof of the theorem is now complete.

At this stage, it should be noted that because of Eq. (3.10) and the Bianchi equations (3.14), the fluid expansion θ is zero if and only if $\bar{\rho} - \mu = 0$, for the case when the fluid is shear-free. However we have shown the stronger result that $\rho = \mu = 0$. These extra conditions may be interpreted as imposing additional constraints on the kinematical quantities of the v_a congruence.[15]

Before proceeding to the proof of the Corollary, we give a summary of the above results, in terms of the spin coefficients, together with the remaining NP equations (4.2) and Bianchi identities (in the tetrad where $\bar{\alpha} + \beta$ is real):

$$\sigma = \lambda = \rho = \mu = \epsilon = \gamma = \tau + \pi = 0, \tag{3.57a}$$

$$\tau^2 + \kappa\nu = (\kappa + \tau)(\alpha - \beta), \tag{3.57b}$$

$$\kappa + \nu = 2(\alpha + \beta), \quad \kappa + \tau = (\alpha + \beta)(1 + 3\dot{p}), \tag{3.57c}$$

$$\Phi_{11} = \kappa(\alpha - \beta), \quad \Psi_4 = 4(\alpha + \beta)(\alpha - \beta),$$

$$\Lambda = \tau(\beta - \alpha), \tag{3.57d}$$

$$2(\alpha + \beta)^2\{(1 + 3\dot{p})(3\dot{p} - 1) + 9\ddot{p}(w + p)\} + \Psi_4(1 + 3\dot{p}) = 0, \tag{3.57e}$$

$$\delta\kappa = \kappa(\alpha + 3\beta + 2\tau), \tag{3.57f}$$

$$\delta\nu = \nu(2\tau - 3\alpha - \beta) + \Psi_4, \tag{3.57g}$$

$$\delta\tau = \tau(\tau - \alpha + \beta) - \kappa\nu, \tag{3.57h}$$

$$\delta(\alpha - \beta) = (\alpha - \beta)(\alpha - \beta - \tau + \kappa), \tag{3.57i}$$

$$\delta(\alpha + \beta) = (\alpha + \beta)(2\tau - 2\nu + 3\alpha + \beta), \tag{3.57j}$$

$$\delta\Psi_4 = \Psi_4(\tau - 4\beta + 3\kappa), \tag{3.57k}$$

$$\delta w = 3(w + p)(\alpha + \beta), \tag{3.57l}$$

where D and Δ derivatives of Ψ_4 and w and all spin coefficients are zero.

The NP commutators (4.4), as applied to Eqs. (3.57f)–(3.57l), are now identically satisfied by the above system (3.57). There remains to consider the δ operator applied to Eqs. (3.57b)–(3.57e). We find that nothing new is obtained from Eqs. (3.57c) and (3.57d) when this differentiation is carried out, but that Eq. (3.57e) leads to[16]

$$\kappa + 3\tau = (\alpha + \beta)S(w), \tag{3.58}$$

where

$$S(w) := 2 - 3\dot{G}\{w + p\}/G. \tag{3.59}$$

Equations (3.57c) and (3.58) imply

$$2\kappa = (\alpha + \beta)(3 + 9\dot{p} - S), \tag{3.60}$$

$$2\tau = (\alpha + \beta)(S - 1 - 3\dot{p}), \tag{3.61}$$

which together with Eqs. (3.57d) give

$$\Phi_{11}(S - 1 - 3\dot{p}) = \Lambda(S - 3 - 9\dot{p}). \tag{3.62}$$

This is a nonlinear, third-order differential equation for $p(w)$. It follows from Eqs. (3.57c) and (3.60) that

$$2\nu = (\alpha + \beta)(1 - 9\dot{p} + S). \tag{3.63}$$

Thus, using Eqs. (3.57d), (3.57e), (3.60), (3.61), and (3.63), Eq. (3.57b) reduces to

$$2(S - 1 - 3\dot{p})^2 + 2(1 - 9\dot{p} + S)(3 + 9\dot{p} - S) + G(1 + 3\dot{p}) = 0, \tag{3.64}$$

which is a nonlinear, third-order differential equation for $p(w)$. Finally, applying the δ operator to Eq. (3.60) leads to the nonlinear, fourth-order equation

$$(3 + 9\dot{p} - S)(4 - 36\dot{p} + 4S + G) = 12(w + p)(9\ddot{p} - \dot{S}). \tag{3.65}$$

Equations (3.62), (3.64), and (3.65), which must all be simultaneously satisfied by $p(w)$, express the total remaining integrability conditions, at this level, for the system (3.57). In order that solutions to Einstein's field equations, subject to the indicated assumptions, exist, we must show that a choice of $p(w)$ can be made so that Eqs. (3.62), (3.64), and (3.65) can be simultaneously satisfied. Remarkably, we will show that solutions do, in fact, exist by essen-

tially "reducing" these equations to a *single*, nonlinear, second-order differential equation.

We proceed by first solving Eq. (3.62) for S, yielding

$$S := 2 - 3\dot{G}(w+p)/G$$
$$= (1+3\dot{p})(\Phi_{11} - 3\Lambda)/(\Phi_{11} - \Lambda). \quad (3.66)$$

Substituting this expression for S into Eq. (3.64) leads to

$$8\{\Phi_{11} - \Lambda - 3\dot{p}(\Phi_{11} + \Lambda)\} = G(\Lambda - \Phi_{11}), \quad (3.67)$$

or equivalently

$$9(w+p)(w+3p-2K)\ddot{p}$$
$$= (1+3\dot{p})(9\dot{p}w + 18\dot{p}K - 9\dot{p}p - w - 3p + 2K). \quad (3.68)$$

A simple check shows that $\dot{p} = \text{const}$ is not a solution of the system (3.65)–(3.67). Thus necessarily $\dot{p} \neq \text{const}$ which implies $\Lambda \neq \Phi_{11}$. If Eq. (3.68) is solved for $\ddot{p}$ then by differentiating, an expression for $\dddot{p}$ is obtained. When we substitute this expression for $\dddot{p}$ and the one for $\ddot{p}$ as obtained from Eq. (3.68), into Eq. (3.66), there results an identity. Similarly, we may use Eq. (3.66) to eliminate S and $\dot{S}$ in Eq. (3.65) thereby yielding a second-order differential equation. Finally, if the expression for $\ddot{p}$, as determined from Eq. (3.68), is substituted into this equation, an identity results.[17] Thus we conclude that any solution of Eq. (3.68) satisfies Eqs. (3.65) and (3.66). This completes the proof of the Corollary.

In general, for shear-free, type N space-times with $p = p(w)$ it follows from Eqs. (3.57), that the fluid[18] has nonzero acceleration and vorticity:

$$\dot{u}_a = -3\dot{p}(\alpha+\beta)\{m_a + \bar{m}_a\} \neq 0, \quad (3.69)$$
$$\omega_a = i(\alpha+\beta)\{\bar{m}_a - m_a\} \neq 0. \quad (3.70)$$

Thus $\dot{u}_a \omega^a = 0$, and therefore the acceleration vector is orthogonal to the vorticity vector. This is to be compared with the complementary results obtained by White and Collins[6] where they consider the case when the vorticity vector is parallel to the acceleration. They find that if $\omega_a \neq 0$ then necessarily $\theta = 0$ and all possible space-times[19] are either Petrov type I or type D.

IV. DISCUSSION

In some of the more recent studies devoted to shear-free fluids, an orthonormal tetrad formalism was employed. This approach does appear enticing because of the ease of adapting this tetrad to the kinematic features of the fluid. This appeal is further enhanced when additional assumptions, of certain special alignment conditions, are imposed on the fluid kinematic quantities.[6] However, the present work does suggest that the role of null congruences should be considered, especially when the Weyl tensor is algebraically special. (In this case, it seems natural to adapt the null tetrad to certain features of the fluid as well as the Weyl tensor, by, possibly, aligning one of the null vectors along the repeated principal null direction of the Weyl tensor and then using some of the remaining freedom to require that the two-space defined by the null tetrad vectors l and n contain the fluid four-velocity vector.) Indeed, it could prove interesting to reexamine some of the above cited work within the context of null tetrads because the proof of the conjecture, if true, might ultimately be obtained by a division of labor between the two approaches.

We intend to continue the analysis of shear-free fluids by systematically examining all remaining algebraically special space-times. As a final point, another avenue for future study, as suggested by the above results, is to consider shear-free fluids where the vorticity vector is orthogonal to the acceleration.[19]

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APPENDIX: SPECIALIZATION OF TETRAD

We consider the commutator $[\Delta, D]$ applied to w, which in conjunction with Eqs. (3.12), (3.14), (3.15), and (3.26), leads to

$$(D-\Delta)\rho = 2\{(\tau+\bar{\pi})(\alpha+\bar{\beta}) + (\bar{\tau}+\pi)(\bar{\alpha}+\beta)\}. \quad (A1)$$

Applying the $\bar{\delta}$ operator to Eq. (3.12b) yields

$$\bar{\delta}(\bar{\alpha}+\beta) = (\bar{\alpha}+\beta)(\alpha - \bar{\beta} + \bar{\tau} + \nu)$$
$$+ (\alpha+\bar{\beta})(\kappa + \bar{\pi} + 2\tau - 2\bar{\nu}), \quad (A2)$$

while δ applied to Eq. (3.12d) leads to

$$\bar{\delta}(\bar{\alpha}+\beta) = (\bar{\alpha}+\beta)(2\bar{\tau} - \pi + \alpha - \bar{\beta} + 3\bar{\kappa})$$
$$+ (\alpha+\bar{\beta})(\tau - \bar{\nu} + 2\bar{\pi} - 2\kappa). \quad (A3)$$

Comparison of (A2) and (A3) gives

$$\kappa(\alpha+\bar{\beta}) = \bar{\kappa}(\bar{\alpha}+\beta), \quad (A4)$$

where use has been made of Eqs. (3.12). Since the rotation (3.7) induces the transformation

$$\bar{\bar{\alpha}} + \bar{\beta} = e^{i\xi}(\bar{\alpha}+\beta), \quad (A5)$$

we may choose a tetrad in which

$$\bar{\alpha} + \beta = \alpha + \bar{\beta}. \quad (A6)$$

It then follows, in the tetrad where $\bar{\alpha}+\beta$ is real, that

$$\kappa = \bar{\kappa}, \quad \epsilon = \bar{\epsilon}, \quad \pi = \bar{\pi}, \quad \gamma = \bar{\gamma},$$
$$\bar{\nu} - \nu = \tau - \bar{\tau}, \quad \Psi_4 = \bar{\Psi}_4. \quad (A7)$$

Equations (3.16) and (A2) now imply

$$\Psi_4 = 2(\bar{\alpha}+\beta)(\kappa + \bar{\tau} + \nu + \pi - 4\bar{\beta}), \quad (A8)$$

and consequently

$$2(\bar{\beta} - \beta) = \nu - \bar{\nu} = \bar{\tau} - \tau. \quad (A9)$$

However, using the NP equations (4.2a) and (4.2b), and noting that κ and ρ are real, leads to

$$\kappa\{\bar{\tau} - \tau + 2(\bar{\beta} - \beta)\} = 0, \quad (A10)$$

which together with Eq. (A9) gives

$$\beta = \bar{\beta}. \tag{A11}$$

We now readily conclude that α, ν, and τ must be real.

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On a Weyl-type theorem for higher-order Lagrangians

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Weyl's theorem is extended making use of the theory of concomitants to obtain a Lagrangian density for the massless bosonic fields without dimensional constants. It turns out to be quadratic in the gravitational field and encompasses all the theories that usually appear in the literature. It is shown that the gauge invariance of the Lagrangian follows from the invariance of the field equations.

I. INTRODUCTION

Weyl's theorem[1] establishes that the most general Lagrangian density that may be constructed with the metric and its derivatives up to second order which is linear in second derivatives is $a\sqrt{-g}R + b\sqrt{-g}$. This Lagrangian is the basis of general relativity (GR). But the difficulties that appear when one tries to quantize this theory have induced many researchers to correct it in different ways (increasing its order or degree, adding new bosonic or fermionic fields, and so on) to solve these problems.

The troubles of the quantization of the Einstein action are well known. It is usually believed that they are originated in the fact that if we want a dimensionless action linear in the scalar curvature, then the Lagrangian has a dimensional constant.[2,3] On the other hand, those theories that may be quantized successfully in the usual way all have dimensionless constants and come from Lagrangian densities that are quadratic in the fields.

One way to try to solve the problem is to replace the dimensional constant by fields as was first proposed by Brans and Dicke and followed, for example, by Batakis.[4] Another way is to begin with a theory without dimensional constants and then to make gravity an effective theory where the dimensional constant appears by Feynman integration over dimensional fields.[5] [A similar method is followed to obtain the Yukawa potential from the gauge theory of $SU(2)\times U(1)$ groups.] Another well-known approach is supergravity.[3] It is also known that when one uses an adequately constructed quadratic Lagrangian for gravity, at least the semiclassical theory that is obtained from it turns out to be renormalizable.[6]

Therefore for all that has been expressed, we think it is interesting to generalize somehow Weyl's theorem to study, at least, the problems of the last type of theories. Thus the purpose of this work is to obtain in a rigorous way the quadratic Lagrangians that are usually used for semiclassical gravity (or eventually more general ones: we do not ask them to be *a priori* quadratic in the Riemann tensor) using arguments as those used to deduce Weyl's theorem and the theory of concomitants which it originated, but including the hypothesis of nondimensionality of the constants which they did not use, together with the uniqueness of the Einsten tensor proved by Cartan.[7]

We also want to show the form of the Lagrangian terms for other fields coupled to the gravitational one with allowed interactions, always imposing dimensional constants not to be present. Then any of the fields could become constant, if necessary, to generate dimensional constants as in the Brans–Dicke theory. For the sake of simplicity, we only deal with bosonic massless fields in this first stage, i.e., spin-0, -1, and -2 fields, leaving the treatment of fermionic spin-$\frac{1}{2}$ and -$\frac{3}{2}$ fields for a forthcoming paper.

We also prove that, for this general Lagrangian, the gauge invariance of the field equations (a mandatory hypothesis since they have physical meaning) implies the gauge invariance of the Lagrangian itself, restricting thus severely its general form.

II. THE LAGRANGIAN DENSITY FOR THE BOSONIC FIELDS

The aim of this work is to find in a rigorous way the Lagrangian density for a theory that fulfills the conditions below.

(i) The fields involved are the metric g_{ij}, the electromagnetic potential vector A_i, and a scalar field φ. The latter will play different roles, in general the one of an ordinary field or eventually a constant.

(ii) Dimensional constants are not allowed because

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they introduce well-known problems yielding generally nonrenormalizable theories.

(iii) The Lagrangian will contain only the derivatives that appear in Eq. (1). We introduce only first derivatives of A_i and φ because we want second-order field equations for these fields. On the contrary, we allow first- and second-order derivatives of g_{ij} because naturally we want GR to be contained in our general theory. (Remember that the Hilbert action is degenerate, so the field equations are of second order even if the Lagrangian has the same order.) Besides, we do not impose any maximum degree to the gravitational field in the Lagrangian.

(iv) Units: We set $c=\hbar=1$. The action is dimensionless so to be able to construct the generating functional. Therefore

$$[S]=1 \quad \text{and} \quad [g_{ij}]=1.$$

Then

$$[L]=l^{-4}, \quad [\varphi]=[A_i]=l^{-1},$$

and

$$[\kappa]=l^{-1}, \quad \text{with } \kappa^2=16\pi G,$$

where G is the Newtonian constant.

(v) We require gauge invariance of the electromagnetic field equations.

So let L be a Lagrangian concomitant of the metric tensor, the electromagnetic potential (i.e., in a precise mathematical language a convector), a scalar field, and their derivatives up to the following order:

$$L=L(g_{ij};g_{ij,h};g_{ij,hk};A_i;A_{i,j};\varphi;\varphi_{,j}). \tag{1}$$

From condition (iii) and field dimensions (iv), by a change of scale λ in L, we will have

$$L(g_{ij};\lambda g_{ij,h};\lambda^2 g_{ij,hk};\lambda A_i;\lambda^2 A_{i,j};\lambda\varphi;\lambda^2\varphi_{,i})$$
$$=\lambda^4 L(g_{ij};g_{ij,h};g_{ij,hk};A_i;A_{i,j}\varphi;\varphi_{,i}).$$

Differentiating four times with respect to λ, making $\lambda\to 0$ and applying the replacement theorem,[8] we obtain

$$\begin{aligned}L=&\Lambda_1^{ijhk}R_{ijhk}\varphi^2+\Lambda_1^{ijhks}R_{ijhk}A_s\varphi+\Lambda_2^{ijhks}R_{ijhk}\varphi_{,s}\\&+\Lambda_1^{ijhkrs}R_{ijhk}A_rA_s+\Lambda_2^{ijhkrs}R_{ijhk}A_{r;s}+\Lambda_1\varphi^4\\&+\Lambda_1^iA_i\varphi^3+\Lambda_2^i\varphi^2\varphi_{,i}+\Lambda_1^{ij}\varphi^2A_iA_j+\Lambda_2^{ij}A_{i;j}\varphi^2\\&+\Lambda_3^{ij}\varphi\varphi_{,i}A_j+\Lambda_4^{ij}\varphi_{,i}\varphi_{,j}+\Lambda_1^{ijk}\varphi A_iA_jA_k\\&+\Lambda_2^{ijk}\varphi A_iA_{j;k}+\Lambda_2^{ijhk}A_iA_jA_hA_k+\Lambda_3^{ijhk}A_iA_jA_{h;k}\\&+\Lambda_4^{ijhk}A_{i;j}A_{h;k}+\Lambda_1^{ijhklmst}R_{ijhk}R_{lmst},\end{aligned} \tag{2}$$

where $\Lambda_t^{\cdots}=\Lambda_t^{\cdots}(g_{ij})$ are tensorial densities, R_{ijhk} is the Riemann tensor, and ; stands for covariant differentiation with respect to the Christoffel symbols Γ_{jk}^i.

Recently, the $\Lambda_t^{\cdots}(g_{ij})$ have been determined for any order of the tensor.[9,10] According to those results and taking into account that $n=4$, n being the space-time dimension, we can say that

(i) $\Lambda=$ const,

(ii) $\Lambda^i=0$,

(iii) $\Lambda^{ij}=a\sqrt{-g}g^{ij}$,

(iv) $\Lambda^{ijh}/\sqrt{-g}$, is a linear combination of $g^{[ij}g^{hk]}$ and ϵ^{ijhk},

where [ ] indicates the set built up from the permutation of all indexes included in [ ]. For example,

$$g^{[ij}g^{hk]}=\{g^{ij}g^{hk},g^{ih}g^{jk},g^{ik}g^{jh}\},$$

(v) $\Lambda^{ijh}=0$,

(vi) $\Lambda^{ijhkl}=0$,

(vii) $\Lambda^{ijhklm}/\sqrt{-g}$ is a linear combination of $g^{[ij}g^{hk}g^{lm]}$ and $g^{[ij}\epsilon^{hklm]}$,

(viii) $\Lambda^{ijkhlmst}/\sqrt{-g}$ is a linear combination of $g^{[ij}g^{hk}g^{lm}g^{st]}$ and $g^{[ih}g^{jk}\epsilon^{lmst]}$.

So we obtain the following expression for the action:

$$\begin{aligned}S=\int L\,d^4x=\int\sqrt{-g}\{&a_1\varphi^2R+a_2RA^iA_i\\&+a_3R^{ij}A_iA_j+a_4R^{ij}A_{i;j}+a_5\varphi^4+a_6\varphi^2A^iA_i\\&+a_7\varphi\varphi_{,i}A^i+a_8\varphi_{,i}\varphi^{,i}+a_9A^iA^jA_{i;j}+a_{10}F_{ij}F^{ij}\\&+a_{11}A_{i;j}A^{i;j}+a_{12}R^2+a_{13}R_{ijhk}R^{ijhk}\\&+a_{14}R_{ijhk}R^{ihjk}+a_{15}R_{ij}R^{ij}+a_{16}\epsilon^{ijhk}R_{ij}{}^{lm}R_{hklm}\\&+a_{17}\epsilon^{ijhk}R_{iljm}R_{hk}{}^{lm}+\text{total divergence}\}d^4x,\end{aligned} \tag{3}$$

where R_{ij} the Ricci tensor, R the scalar curvature, and $F_{ij}=A_{i;j}-A_{j;i}$.

Let us suppose that $E(L)=\delta S/\delta\varphi$ is gauge invariant. Then $\partial E(L)/\partial A_m=0$, which implies that

$$4a_6\varphi A_ig^{im}-a_7\Gamma_{th}^t\varphi g^{hm}+a_7\varphi g^{ht}g^{ms}g_{ts,h}=0. \tag{4}$$

Differentiating Eq. (4), with respect to A_i, it turns out immediately that $a_6=0$. Then contracting Eq. (4) with g_{mk} and differentiating with respect to $g_{ab,c}$, it gives

$$a_7\varphi\{g^{bc}\delta^a{}_k-g^{ab}\delta^c{}_k+g^{ac}\delta^b{}_k\}=0.$$

Multiplying by g_{bc} and contracting a with k, we obtain that $a_7=0$.

Let us suppose now that $E^r(L)=\delta S/\delta A_r$ is gauge invariant. Then $\delta E^r(L)/\partial A_m=0$, that is,

$$\begin{aligned}&2a_2Rg^{mr}+2a_3R^{mr}+2a_6\varphi^2g^{mr}+a_9\{A_{i;j}g^{im}g^{jr}\\&-2\Gamma_{ij}^rA_hg^{ih}g^{jm}-2\Gamma_{ij}^mA_hg^{ih}g^{jr}-2\Gamma_{ij}^tA_tg^{im}g^{jr}\\&-\Gamma_{ts}^tA_kg^{rm}g^{sk}-\Gamma_{ts}^tA_hg^{rh}g^{sm}-A_{k;s}g^{rm}g^{sk}\\&+A_kg^{ri}g^{mj}g^{sk}g_{ij,s}+A_hg^{ri}g^{hj}g^{sm}g_{ij,s}\\&+A_kg^{si}g^{kj}g^{rm}g_{ij,s}+A_hg^{si}g^{mj}g^{rh}g_{ij,s}\}\\&+a_{11}\{2\Gamma_{ij}^m\Gamma_{hk}^rg^{ih}g^{jk}+2\Gamma_{ls}^l\Gamma_{hk}^mg^{rh}g^{sk}+2\Gamma_{hk,s}^mg^{rh}g^{sk}\\&-2\Gamma_{hk}^mg^{ri}g^{hj}g^{sk}g_{ij,s}-2\Gamma_{hk}^mg^{rh}g^{si}g^{kj}g_{ij,s}\}.\end{aligned} \tag{5}$$

Differentiating Eq. (5), with respect to $g_{ab,cd}$, taking at the point under consideration a basis, where $g_{ij}=\text{diag}(1-1-1-1)$ and making $m=a=b=c=1$, $r=d=2$, $a_{11}=0$ results. Taking $m=c=2$, $r=a=3$, and $b=d=4$, then $a_3=0$. And making $d=c=1$, $m=r=a=b=2$, $a_2=0$ results.

Differentiating Eq. (5) with respect to $A_{a,b}$ and taking into account that $a_2=a_3=a_{11}=0$,

$$a_9(g^{am}g^{br}-g^{rm}g^{ab})=0$$

results. Letting $a=b=1$, $r=m=2$, we get $a_9=0$.

Let us finally suppose that $E^{ij}(L)=\delta S/\delta g_{ij}$ is gauge

invariant, then $\partial E^{ij}(L)/\partial A_m = 0$. It is clear due to what we have just seen that this is the same as

$$\frac{\partial E^{ij}(L_4)}{\partial A_m} = 0, \quad \text{where } L_4 = a_4\sqrt{-g}R^{ij}A_{i;j}.$$

As L_4 is linear in $g_{ij,hk}$, fourth-order derivatives do not appear in $E^{ij}(L_4)$. Differentiating $\partial E^{ij}(L_4)/\partial A_m$ with respect to $g_{kl,hsc}$ and then contracting with $g_{st}g_{ah}g_{ck}$, it results, after a long computation, that $a_4 = 0$. So we have proved the following.

Theorem: If L is a Lagrangian density of the form

$$L = L(g_{ij};g_{ij,h};g_{ij,hk};A_i;A_{i,j};\varphi;\varphi_{,i}),$$

which satisfies hypotheses (i)–(v), then gauge invariance of the associated Euler–Lagrange equations implies gauge invariance of the Lagrangian and it becomes

$$\begin{aligned} L = {} & b_1\sqrt{-g}R\varphi^2 + b_2\sqrt{-g}\varphi^4 + b_3\sqrt{-g}\varphi_{,i}\varphi_{ij}g^{ij} \\ & + b_4\sqrt{-g}F_{ij}F^{ij} + b_5\sqrt{-g}R^2 + b_6\sqrt{-g}R_{ijhk}R^{ijhk} \\ & + b_7\sqrt{-g}R_{ij}R^{ij}. \end{aligned} \tag{6}$$

Note that $b_5\sqrt{-g}R^2$, $b_6\sqrt{-g}R_{ijhk}R^{ijhk}$, and $b_7\sqrt{-g}R_{ij}R^{ij}$ terms may be related through the Gauss–Bonnet theorem.

III. SOME CONSIDERATIONS ON THE CONSTRUCTED LAGRANGIAN

Now we can reobtain several well-known classical theories from the Lagrangian of Eq. (6) choosing different values for the constants.

(a) General relativity: General relativity is a particular case of Eq. (6) avoiding dimensional constants as in the Brans–Dicke theory[11] whose Lagrangian may be written

$$L = -\sqrt{-g}\{-\varphi^2 R + 4w g^{ij}\varphi_{,i}\varphi_{,j}\},$$

w being a numerical constant. This is obtained from our Eq. (6) taking $b_1 = -\frac{1}{2}$, $b_3 = 4w$, and all other coefficients equal to zero. Finally, the Einstein Lagrangian is obtained setting $\varphi^2 = \kappa^{-2}$.

(b) Maxwell–Einstein: The electromagnetic field is minimally coupled to the gravitational field replacing all partial derivatives which appear in its formulation in Minkowskian space-time by covariant ones. Maxwell electromagnetism plus relativity can be obtained from Eq. (6) making $b_1 = -\frac{1}{2}$; $b_4 = 2\pi/137$; all other $b_i = 0$ and thinking of φ^2 as κ^{-2}.

(c) Scalar field Lagrangians: It is widely accepted that the Lagrangian for the massless scalar self-interacting field in curved space-time is

$$L = \xi\varphi^2\sqrt{-g}R + \sqrt{-g}g^{ij}\varphi_{,i}\varphi_{,j} + \sqrt{-g}\lambda\varphi^4.$$

So we must take in Eq. (6) $b_1 = \xi, b_2 = \lambda, b_3 = 1$, with $\xi = 0$ or $\frac{1}{6}$ for minimal or conformal coupling, respectively, and all other coefficients $b_i = 0$. With two different scalar fields we could also add the $\kappa^{-2}\sqrt{-g}R$ term to obtain GR coupled to the matter scalar field.

(d) Quadratic Lagrangian for the gravitational field: In spite of the fact that predictions based on Einstein's relativity are in large agreement with experience, it is necessary to form a generalization for high energies—high curvatures—which could circumvent its quantum difficulties. Quantum field theories in curved space-time take into account the quantum properties of matter, including the eventual perturbations of the metric due to back reaction, but they do not quantize the background geometry which remains as a classical external field. The results obtained by this procedure—although incomplete—would eventually represent some semiclassical limit of a more general theory where the space-time geometry would be quantized too. We believe this limit describes the physical phenomena in those regions that verify $\max(|R^{ij}{}_{hk}|) < c^3/16\pi G\hbar \equiv l_p^{-2}$, where l_p is the Planck longitude, $l_p \sim 10^{-32}$ cm.

The pure gravitational terms of the Lagrangian of Eq. (6)—with the identification of $b_1\varphi^2$ with κ^{-2} and $b_2\varphi^4$ with Λ, Λ the cosmological constant—are those generally used by the quantum field theory in curved space-time. Its action for gravitation is

$$S_g = \int \sqrt{-g}\{(R/2\kappa^2 - 2\Lambda) + \alpha R^2 + \beta R_{ij}R^{ij}\}d^4x$$

obtained by taking $b_1 = 1$, $b_2 = -2$, $b_3 = \alpha$, $b_7 = \beta$ in our Eq. (6) and making use of the Gauss–Bonnet theorem.

Besides its quantum interest, the quadratic Lagrangian theories may give information about classical features of space-time for high curvatures. For example, we can consider the theory with Lagrangian $L = \{(R/2\kappa^2 - 2\Lambda) + \alpha R^2\}\sqrt{-g}$ that can be obtained from our Eq. (6) making $b_1 = 1$, $b_2 = -2$, $b_5 = \alpha$, and all other $b_i = 0$. These kinds of theories are studied in Ref. 12 where it is shown that black holes have no hair as it is in ordinary GR.

Our Lagrangian density also contains the action which Strominger shows to have non-negative energy for asymtotically flat limits[13] if we choose $F_{ij} = 0$, $b_1\varphi^2 = 1$, $b_5 = \frac{1}{2}\beta^2$, and all other $b_i = 0$.

IV. CONCLUSIONS

We have extended Weyl's theorem, making use of the theory of concomitants that comes from it, to obtain a Lagrangian density for the massless bosonic fields, without dimensional constants. It turns out quadratic in the gravitational field even if this order was not prescribed from the outset. This circumvents, at least at the semiclassical level, the quantum difficulties of the Einstein Lagrangian that comes from the original Weyl theorem. We have also limited the possible couplings among the bosonic matter fields and among them and the metric, choosing only Lagrangians with no dimensional constants.

Moreover, we have shown that it is not necessary to ask the Lagrangian to be gauge invariant because its invariance follows from the invariance of the field equations. This also excludes interactions which would be allowed if we only took into account tensorial concomitants and dimensional analysis.

The Lagrangian density thus obtained encompasses all theories that usually appear in the literature as we have shown in Sec. III.

In a forthcoming paper this work will be extended to

include fermionic fields, making use of spinorial concomitants, allowing us to compare the results not only with GR but also with supergravity theories.

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The stochastic Wigner–Weisskopf atom

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Using techniques of quantum stochastic calculus, a dilation scheme is developed to describe the evolution of a two-level atom, which is initially in a (nontracial) Gibbs state, through a radiation field. The Wigner–Weisskopf approximation is assumed but not the rotating wave approximation, the latter being shown to be equivalent to the requirement that the dilation satisfies the quantum detailed balance condition with respect to the initial state.

I. INTRODUCTION

The quantum mechanical description of the interaction between radiation and matter has been treated extensively (see, e.g., Refs. 1 and 2) by formal mathematical techniques bearing a strong "family resemblance"[3] to those of stochastic analysis (e.g., Ref. 4). Specifically, the radiation field is regarded as a heatbath into which atomic systems diffuse under the influence of the interaction.

Recently, Hudson and Parthasarathy[5] have developed a theory of quantum stochastic calculus which is formulated intrinsically within the framework of the mathematics of second quantization. Accardi[6] applied this calculus to describe the diffusion of a two-level atom into a radiation field and demonstrated that the results of previous analyses by von Waldenfels[7] could be interpreted in terms of a stochastic differential equation of the Hudson–Parthasarathy type. Further investigations of the structure of this equation were carried out by Maassen.[8] The behavior of the radiation field as "quantum noise" is described in terms of the quantum Brownian motion process of Ref. 9 and arises through the Wigner–Weisskopf approximation wherein the finite number of interacting modes of the field is replaced by a boson system with infinitely many degrees of freedom.

All the above analyses have employed a device called the rotating wave approximation whereby those terms in the interaction Hamiltonian that fail to commute with the total number operator of the atom and the field are consigned to oblivion. The main aim of this paper is to demonstrate that the techniques of quantum stochastic calculus are sufficiently powerful as to enable us to dispense with this procedure. An alternative approach to this problem, based on the weak coupling limit, can be found in Refs. 10 and 11. In that approach it is shown that the rotating wave approximation is reliable only when the natural frequency w_0 of the two-level atom is large in comparison with the rate of damping imparted by the radiation field.

The plan of this article is as follows. In Sec. II we review those results of algebraic quantum field theory we will use in the sequel. Section III describes the application of quantum stochastic calculus to dilating a dynamical semigroup on a von Neumann algebra to an automorphism group of a "bigger" von Neumann algebra. This is, to some extent, the quantum theoretic analog of a diffusion process. In physical terms, the irreversible evolution of an atomic system S within some environment $\hat{S}$ is described by projection of the reversible evolution of the combined system and environment $(S+\hat{S})$.

In our case, S is a two-level atom and $\hat{S}$ the radiation field. We describe their interaction in Sec. IV and show in Sec. V how the Wigner–Weisskopf approximation leads naturally to a description of the dynamics of the interaction in terms of a stochastic dilation, as described above. We refer to this dilation scheme for the two-level atom as "the stochastic Wigner–Weisskopf atom." In Sec. VI we discuss some of the properties of the dynamical semigroup describing the irreversible evolution of the atom and prove, in particular, that its stochastic dilation is stationary with respect to given equilibrium states on S and $\hat{S}$ if and only if the rotating wave approximation is made.

We employ the following notation; if h is a complex separable Hilbert space then $\bar{h}$ denotes its dual.

If T is a densely defined operator on h, we define $\overline{T}$ on $\bar{h}$ by the prescription

$$\overline{T}\bar{f} = \overline{Tf}$$

whenever f lies in the domain of T.

If T is a closable operator on h, we denote its closure by T^c.

Any proposition containing the symbol $T^{\#}$ should be read twice, once in which $T^{\#}$ is read as T, and once in which it is read as T^*.

If V_1 and V_2 are complex vector spaces then $V_1 \otimes V_2$ denotes their (algebraic) tensor product.

We will work in a system of units in which Boltzmann's constant is 1 and Planck's constant is 2π.

II. PRELIMINARIES—ALGEBRAIC DESCRIPTION OF THE FREE BOSON FIELD IN THERMAL EQUILIBRIUM[12]

Let $\Gamma(h)$ denote boson Fock space over the complex separable Hilbert space h and Ω be the vacuum vector in $\Gamma(h)$. For each $f \in h$, let $b(f)$, $b^\dagger(f)$ denote, respectively, the annihilation and creation operators on $\Gamma(h)$, these being mutually adjoint on the dense domain provided by the linear span of $\{w(f)\Omega,\ f \in h\}$, where the Weyl operator $w(f) = \exp[(b^\dagger(f) - b(f))^c]$.

Let $C(h)$ be the (polynomial) CCR algebra over h, i.e., the complex, involutive algebra with identity I generated by $\{a(f), f \in h\}$ satisfying

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$$a(f+cg)=a(f)+\bar{c}a(g),$$

$$[a(f),a(g)]=0, \tag{2.1}$$

$$[a(f),a^{\dagger}(g)]=\langle f,g\rangle I,$$

for each $f,g\in h$, $c\in\mathbb{C}$.

For $\mu>0$, τ_μ will denote the universally invariant, quasifree state on $C(h)$ whose two-point function is given by

$$\tau_\mu(a^{\dagger}(g)a(f))=\mu^2\langle f,g\rangle, \tag{2.2}$$

for each $f,g\in h$. By (2.1) and linearity of τ_μ we have

$$\tau_\mu(a(f)a^{\dagger}(g))=\lambda^2\langle f,g\rangle,$$

where $\lambda=(1+\mu^2)^{1/2}$. For $\alpha>0$ we may write

$$\mu^2=e^{-\alpha}/(1-e^{-\alpha})$$

so that

$$\lambda^2=1/(1-e^{-\alpha})$$

and interpret α as a fixed multiple of an inverse temperature parameter.

We construct a representation π_μ of the algebra $C(h)$ as densely defined operators on the Hilbert space $\mathbf{H}=\Gamma(h)\otimes\Gamma(\bar{h})$, with common invariant domain $\mathbf{D}(h)$, the linear span of

$$\left\{\frac{d^n}{dt_1\cdots dt_n}W\left(f+\sum_{j=1}^{n}t_jg_j\right)\psi_0|_{t_1=\cdots=t_n=0},\right.$$

$$\left.f,g_j\in h,\ t_j\in\mathbb{R},\ 1\leqslant j\leqslant n,\ n\in\mathbb{N}\cup\{0\}\right\},$$

where $\psi_0=\Omega\otimes\bar{\Omega}$ [$\bar{\Omega}$ being the vacuum vector in $\Gamma(\bar{h})$] and $W(f)=w(\lambda f)\otimes w(-\mu\bar{f})$. In particular we have, for each $f\in h$,

$$\begin{aligned}\pi_\mu(a(f))&=\lambda b(f)\otimes I+\mu I\otimes\bar{b}^{\dagger}(\bar{f}),\\ \pi_\mu(a^{\dagger}(f))&=\lambda b^{\dagger}(f)\otimes I+\mu I\otimes\bar{b}(\bar{f}),\end{aligned} \tag{2.3}$$

and the state τ_μ is realized as

$$\tau_\mu(X)=\langle\psi_0,\pi_\mu(X)\psi_0\rangle, \tag{2.4}$$

where $X\in C(h)$.

Let U be a unitary operator on h. We define its second quantization $\Gamma(U)$ by continuous linear extension of the prescription

$$\Gamma(U)W(f)\psi_0=W(Uf)\psi_0. \tag{2.5}$$

It is not difficult to establish that $\Gamma(U)$ extends to a unitary operator on $\mathbf{H}$. Furthermore, if $\{V(t),\ t\in\mathbb{R}\}$ is a strongly continuous unitary representation of $\mathbb{R}$ in h, then $\{\Gamma(V(t)),\ t\in\mathbb{R}\}$ is a strongly continuous, unitary representation of $\mathbb{R}$ in $\Gamma(h)$. Let $\mathbf{N}$ denote the von Neumann subalgebra of $B(\mathbf{H})$ generated by $\{W(f),\ f\in h\}$. The prescription

$$\alpha_t(X)=\Gamma(V(t))X\Gamma(V(t))^* \tag{2.6}$$

for $X\in\mathbf{N}$, $t\in\mathbb{R}$ yields a one-parameter strongly continuous group of automorphisms of $\mathbf{N}$.

Finally we remark that we may define a state τ_0 on $C(h)$ (corresponding to "zero temperature") by taking $\mu=0$ in (2.2). In this case, a single copy of $\Gamma(h)$ suffices to build the representation π_0 on $C(h)$ wherein $\pi_0(a(f))=b(f)$, $\pi_0(a^{\dagger}(f))=b^{\dagger}(f)$, and $\psi_0=\Omega$.

III. STOCHASTIC DILATIONS OF QUANTUM DYNAMICAL SEMIGROUPS

In this section we will take h to be $L^2(\mathbb{R})$. For $t\geqslant 0$, let $f=\chi_{[0,t)}$ in (2.3) and write $A_t=\pi_\mu(a(\chi_{[0,t)}))$, $A_t^{\dagger}=\pi_\mu(a^{\dagger}(\chi_{[0,t)}))$, then the pair of processes $(A,A^{\dagger})$, where $A^{\#}=\{A_t^{\#},\ t\geqslant 0\}$ constitutes quantum Brownian motion of variance $\sigma^2=\lambda^2+\mu^2$ (Ref. 9).

An extensive theory of stochastic analysis with respect to $(A,A^{\dagger})$ has been developed in Refs. 13 and 14. (In the zero temperature case $\mu=0$, the appropriate theory is that of Ref. 5.) One of the central results of this theory is the quantum Itô product formula which ensures that all products of the stochastic differentials dA and $dA^{\dagger}$ vanish with the exception of

$$dA\,dA^{\dagger}=\lambda^2\,dt,\quad dA^{\dagger}\,dA=\mu^2\,dt. \tag{3.1}$$

Let h_0 be a complex, separable Hilbert space and let $\{G(t),\ t\geqslant 0\}$ and $\{H(t),\ t\geqslant 0\}$ denote families of operators in $\mathbf{B}(h_0)$ such that each $H(t)=H(t)^*$ and the maps $t\to G(t)$ and $t\to H(t)$ are uniformly bounded. The following slight generalization (cf. Ref. 15) of results in Ref. 13 yields an interesting class of stochastic differential equations (SDE's) which we will find of some use in the sequel.

Proposition 1: There exists a unique solution to the SDE

$$\begin{aligned}dU=U(&G^{\dagger}(t)dA-G(t)dA^{\dagger}+(iH(t)\\&-\tfrac{1}{2}\lambda^2G^{\dagger}(t)G(t)-\tfrac{1}{2}\mu^2G(t)G^{\dagger}(t))dt),\\ U(0)&=I,\end{aligned} \tag{3.2}$$

with each $U(t)$ a unitary operator on $h_0\otimes\mathbf{H}$ $(t\geqslant 0)$.

We now turn our attention to the notion of a dilation. Let $\{T_t,\ t\geqslant 0\}$ be a (norm continuous) quantum dynamical semigroup on $B(h_0)$ of finite Lindblad type[16] so that $T_t=\exp tL$ with Ref. 17, for $X\in\mathbf{B}(h_0)$,

$$L(X)=\sum_{j=1}^{N}\left(V_j^*XV_j-\frac{1}{2}\{V_j^*V_j,X\}\right)+i[h,X], \tag{3.3}$$

where $N\in\mathbb{N}$, $V_j\in B(h_0)$ $(1\leqslant j\leqslant N)$, and $h\in B(h_0)$ with $h=h^*$.

A dilation[18] of $(B(h_0),\{T_t,\ t\geqslant 0\})$ is a triple $(M,P,\{\hat{T}_t,\ t\in\mathbb{R}\})$, where M is a von Neumann algebra, P is a projection from M onto $\mathbf{B}(h_0)$ and $\{\hat{T}_t,\ t\in\mathbb{R}\}$ is a strongly continuous, one-parameter group of automorphisms of M such that for all $t\geqslant 0$

$$T_t=P\circ\hat{T}_t\circ l, \tag{3.4}$$

where the injection $l\colon B(h_0)\to M$ is the right inverse of P.

Quantum stochastic calculus yields a universal construction for generating such dilations.[5,8,13,19,20] In this paper we are concerned only with a particular case of the general formula (3.3) and we will now describe its dilation. Indeed the generator of interest has $N=2$ in (3.3) with $V_1=\lambda G^*$ and $V_2=-\mu G$ for $G\in B(h_0)$ with λ and μ as in Sec. II.

The prescription for the dilation is then

$$M=B(h_0)\otimes\mathbf{N}.$$

Here P acts by continuous, linear extension of

$$P(X\otimes Y)=X\langle\psi_0,Y\psi_0\rangle$$

for $X\in B(h_0)$ and $Y\in\mathbb{N}$ so that $l(X)=X\otimes I$ and

$$\hat{T}_t(Y)=U(t)\alpha_t(Y)U(t)^*,\quad t\geqslant 0,$$
$$=\alpha_t(U(-t)^*YU(t)),\quad t<0, \tag{3.5}$$

for $Y\in M$, where $U(t)$ is the solution of (3.2) with $G(t)$ and $H(t)$ taken as the constant operators $l(G)$ and $l(h)$, respectively, and α_t is the automorphism (2.6) with $V(t)$ the shift in $L^2(\mathbb{R})$, i.e., for $t\in\mathbb{R}$, $f\in L^2(\mathbb{R})$,

$$(V(t)f)(s)=f(s-t). \tag{3.6}$$

A class of dilations of particular interest are stationary dilations.[21] Suppose there exists a faithful, normal state τ^0 on $B(h_0)$ so that

$$\tau^0(X)=\operatorname{tr}\rho X$$

for each $X\in B(h_0)$, where ρ is a positive self-adjoint operator on h_0 with $\operatorname{tr}\rho=1$. Suppose also that the semigroup action leaves τ^0 invariant, i.e., for all $t\geqslant 0$,

$$\tau^0(T_t(X))=\tau^0(X) \tag{3.7}$$

for each $X\in\mathbf{B}(h_0)$. In this case, a dilation of $(B(h_0),\{T_t,\ t\geqslant 0\})$ is said to be stationary if there exists a faithful normal state $\tilde{\tau}$ on M such that, for all $t\in\mathbb{R}$, $Y\in M$,

$$\tilde{\tau}(\hat{T}_t(Y))=\tilde{\tau}(Y). \tag{3.8}$$

For the case of interest, we obtain a stationary dilation with $\tilde{\tau}=\tau^0\otimes\tau_\mu$ (Ref. 19) if and only if the semigroup satisfies the quantum detailed balance condition of Ref. 22. The particular form of L ensures that this is equivalent to the requirement[16]

$$\rho^{it}G\rho^{-it}=e^{i\alpha t}G,\quad \rho^{it}h\rho^{-it}=h, \tag{3.9}$$

where α is as in Sec. II.

IV. THE TWO-LEVEL ATOM IN A RADIATION FIELD

From now on, we take $h_0=\mathbb{C}^2$ so that $\mathbf{B}(h_0)$ is the algebra $\mathbf{M}_2(\mathbb{C})$ of 2×2 complex matrices generated (as a $*$-algebra) by the step-down operator

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

which, together with its adjoint, the step-up operator

$$a^*=\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix},$$

satisfies the CAR relations

$$a^2=0,\quad aa^*+a^*a=I. \tag{4.1}$$

The atomic Hamiltonian H_A is given by

$$H_A=\tfrac{1}{2}w_0(a^*a-aa^*),\quad w_0>0,$$

and we associate to the system the Gibbs state at inverse temperature $\beta>0$ with density matrix

$$\rho_A=e^{-\beta H_A}/\operatorname{tr}e^{-\beta H_A}$$
$$=(2\cosh\tfrac{1}{2}\beta w_0)^{-1}\begin{pmatrix}e^{(1/2)\beta w_0} & 0\\ 0 & e^{-(1/2)\beta w_0}\end{pmatrix}. \tag{4.2}$$

The environment of the atom is a system composed of n independent harmonic oscillators which are described by the algebra $C(\mathbb{C}^n)$ generated by $\{a_j,\ 1\leqslant j\leqslant n\}$ satisfying the discrete version of (2.1)

$$[a_j,a_k]=0,\quad [a_j,a_k^\dagger]=\delta_{jk}I\quad (1\leqslant j\leqslant k), \tag{4.3}$$

wherein each $a_j=a(e_j)$ with $\{e_j,\ 1\leqslant j\leqslant n\}$ the natural basis for $\mathbb{C}^n$.

The free Hamiltonian of the environment is

$$H_E=\sum_{j=1}^n w_ja_j^\dagger a_j\quad (w_j>0,\ 1\leqslant j\leqslant n)$$

and we describe it in thermal equilibrium at inverse temperature β by the Gibbs state τ_E, whose density operator is given by

$$\rho_E=e^{-\beta H_E}/\operatorname{tr}e^{-\beta H_E}$$

so that, in particular,

$$\tau_E(a_j)=0=\tau_E(a_j^\dagger)\quad\text{and}\quad \tau_E(a_j^\dagger a_k)=\mu_j^2\delta_{jk}\qquad (1\leqslant j,k\leqslant n), \tag{4.4}$$

where

$$\mu_j^2=e^{-\beta w_j}/(1-e^{-\beta w_j})\quad (1\leqslant j\leqslant n).$$

We take the $*$-representation π_n of $C(\mathbb{C}^n)$ on the Hilbert space $\mathbf{H}_n=\Gamma(\mathbb{C}^n)\otimes\Gamma(\overline{\mathbb{C}}^n)$ whose action on generators is given by

$$\pi_n(a_j)=\lambda_jb(e_j)\otimes I+\mu_jI\otimes\bar{b}^\dagger(\bar{e}_j), \tag{4.5}$$

where $\lambda_j=(1+\mu_j^2)^{1/2}$ $(1\leqslant j\leqslant n)$. We will use the notation $B_j=\pi_n(a_j)$, $B_j^\dagger=\pi_n(a_j^\dagger)$ $(1\leqslant j\leqslant n)$.

States of the combined system and environment will be described by vectors in the Hilbert space $h_0\otimes\mathbf{H}_n$, the interaction between system and environment being given by the Hamiltonian

$$H_I^0=\sum_{j=1}^n g_j(a^*B_j+aB_j)+\bar{g}_j(aB_j^\dagger+a^*B_j^\dagger), \tag{4.6}$$

where the coupling parameters $g_j\in\mathbb{C}$ $(1\leqslant j\leqslant n)$ and we have suppressed the tensor product sign in (4.6) for notational convenience. Here H_I^0 is a densely defined essentially self-adjoint operator on the domain $h_0\otimes\mathbf{D}(\mathbb{C}^n)$.

In previous analyses,[1,2,6,7] the rotating wave approximation is introduced at this stage whereby the contributions of the terms aB_j and $a^*B_j^\dagger$ $(1\leqslant j\leqslant n)$ are eliminated from (4.6) by arguing that at frequencies close to w_j these yield rapid oscillations which average to zero "for times of interest" (Ref. 2, p. 324). Our main purpose in this paper is to study the effect of retaining these terms. In order to keep track of how subsequent results differ from Ref. 6, we introduce a pair of non-negative parameters ϵ and η to measure the contributions of the "antirotating wave" and "rotating wave" terms, respectively.

So in place of (4.6) we study the modified interaction

$$H_I=\sum_{j=1}^n g_j[\epsilon a+\eta a^*]B_j+\bar{g}_j[\epsilon a^*+\eta a]B_j^\dagger. \tag{4.7}$$

Thus the rotating wave approximation is effected by putting $\epsilon=0$ and (4.6) recaptured by the choice $\epsilon=\eta=1$.

Following Refs. 1, 2, 6, and 7 we work in the interaction representation, hence we seek a family of unitary operators on $h_0\otimes\mathbf{H}_n$, $\{W(t),\ t\geqslant 0\}$ satisfying the differential equation

$$\frac{dW(t)}{dt} = -iW(t)K(t), \quad W(0) = I, \tag{4.8}$$

where

$$\begin{aligned} K(t) &= e^{it(H_A + H_E)} H_I e^{-it(H_A + H_E)} \\ &= e^{itH_A}(e^{itH_E} H_I e^{-itH_E}) e^{-itH_A} \\ &= (\epsilon a e^{i\omega_0 t} + \eta a^* e^{-i\omega_0 t}) F(t) \\ &\quad + (\epsilon a^* e^{-i\omega_0 t} + \eta a e^{i\omega_0 t}) F(t)^\dagger, \end{aligned} \tag{4.9}$$

with

$$F(t) = \sum_{j=1}^{n} g_j e^{-i\omega_j t} B_j.$$

From (4.3) and (4.4) we find the following relations hold on the domain $h_0 \otimes D(\mathbb{C}^n)$

$$\begin{aligned} &[F(s), F(t)] = 0, \\ &[F(s), F(t)^\dagger] = \sum_{j=1}^{n} |g_j|^2 e^{-i\omega_j(s-t)}, \end{aligned} \tag{4.10}$$

and

$$\begin{aligned} &\tau_E(F(s)) = 0 = \tau_E(F(s)^\dagger), \\ &\tau_E(F(t)^\dagger F(s)) = \sum_{j=1}^{n} \mu_j^2 |g_j|^2 e^{-i\omega_j(s-t)}, \end{aligned} \tag{4.11}$$

for $s,t \geqslant 0$.

We formally express the solution to (4.8) as a continuous product integral (time ordered exponential)

$$\hat{W}(t) = \prod_0^t \exp(-iK(t))dt. \tag{4.12}$$

V. THE WIGNER–WEISSKOPF APPROXIMATION AND STOCHASTIC EVOLUTION EQUATION

Let us suppose that the ω_j's are distributed over a wide range of frequencies and that the coupling amplitudes $|g_j|$ are all close to a common value $k \geqslant 0$. Under these conditions, it is physically reasonable to make the Wigner–Weisskopf approximation, which, algebraically, is realized as follows. Let $\mathbf{B}$ denote the $*$-subalgebra of $C(\mathbb{C}^n)$ generated by $\{F(t),\ t \geqslant 0\}$ satisfying (4.10). We replace $\mathbf{B}$ by the $*$-algebra, which we denote symbolically as $\partial C(L^2(\mathbb{R}))$, generated by $\{\tilde{F}(t),\ t \geqslant 0\}$ satisfying

$$\begin{aligned} &[\tilde{F}(t), \tilde{F}(s)] = 0, \\ &[\tilde{F}(s), \tilde{F}(t)^\dagger] = k\delta(s-t), \quad s,t \geqslant 0. \end{aligned} \tag{5.1}$$

Furthermore, we consider the state $\tilde{\tau}_E$ on $\partial C(L^2(\mathbb{R}))$ whose one- and two-point functions are given by

$$\begin{aligned} &\tilde{\tau}_E(\tilde{F}(t)) = \tilde{\tau}_E(\tilde{F}(t)^*) = 0, \\ &\tilde{\tau}_E(\tilde{F}(s)\tilde{F}(t)) = \tilde{\tau}_E(\tilde{F}(s)^* F(t)^*) = 0, \\ &\tilde{\tau}_E(\tilde{F}(t)^\dagger F(s)) = k\mu^2 \delta(t-s), \end{aligned} \tag{5.2}$$

for $s,t \geqslant 0$, where $\mu^2 = e^{-\beta\omega_0}/(1 - e^{-\beta\omega_0})$. A discussion of the physical significance of this choice of μ is given in Ref. 7(a). State $\tilde{\tau}_E$ extends from (5.2) onto the whole of $\partial C(L^2(\mathbb{R}))$ in an appropriately quasifree manner [i.e., all higher-order correlation functions[12] are determined by (5.2)].

The relations (5.1) cannot be realized within an operator theoretic framework[23] and so we introduce, for each $f \in L^2(\mathbb{R})$, the "smeared fields"

$$\begin{aligned} A(f) &= (k)^{-1/2} \int_{-\infty}^{\infty} \overline{f(s)} \tilde{F}(s) ds, \\ A^\dagger(f) &= (k)^{-1/2} \int_{-\infty}^{\infty} f(s) \tilde{F}(s)^\dagger ds. \end{aligned} \tag{5.3}$$

From (4.1) and (4.2) we see that $\{A^\#(f), f \in L^2(\mathbb{R})\}$ satisfy (2.1) and $\tilde{\tau}_E$ yields a quasifree state of the form (2.2). Thus, in making the Wigner–Weisskopf approximation, we effectively replace the algebra $C(\mathbb{C}^n)$ acting on $\Gamma(\mathbb{C}^n) \otimes \Gamma(\overline{\mathbb{C}^n})$ through the representation π_n by the algebra $C(L^2(\mathbb{R}))$ acting on $\Gamma(L^2(\mathbb{R})) \otimes \Gamma(\overline{L^2(\mathbb{R})})$ via the representation π_μ.

So writing $A_t = A(\chi_{[0,t)})$, $A_t^\dagger = A^\dagger(\chi_{[0,t)})$, we see that the pair of processes $(A, A^\dagger)$ is precisely quantum Brownian motion of variance σ^2 and furthermore we may formally identify $\tilde{F}(t)dt$ and $\tilde{F}(t)^\dagger dt$, through (5.3), with the stochastic differentials dA and $dA^\dagger$, respectively.

Making this approximation in (4.12) yields a family of unitary operators $\{\hat{W}(t),\ t \geqslant 0\}$ on $h_0 \otimes \mathbf{H}$, where

$$\hat{W}(t) = \prod_0^t \exp(G(t)^* dA - G(t)dA^\dagger) \tag{5.4}$$

with

$$G(t) = i(\epsilon a^* e^{-i\omega_0 t} + \eta a e^{i\omega_0 t})$$

for $t \geqslant 0$. Equation (5.4) is interpreted as a stochastic product integral[5] and is the solution of the SDE

$$\begin{aligned} d\hat{W}(t) &= \hat{W}(t)[G(t)^* dA - G(t)dA^\dagger \\ &\quad - \tfrac{1}{2}(\lambda^2 G^*(t)G(t) + \mu^2 G(t)G^*(t))dt], \\ \hat{W}(0) &= I. \end{aligned} \tag{5.5}$$

Since the $G(t)$'s are clearly uniform bounded, indeed $\|G(t)\| \leqslant \epsilon + \eta$ for all $t \geqslant 0$, Proposition 1 guarantees the existence of a unique solution to (5.5) as an operator valued process on $h_0 \otimes \mathbf{H}$.

Let $V_A(t) = \exp(itH_A)$ denote the free evolution on h_0 ($t \in \mathbb{R}$) and consider the family of unitary operators $\{U(t), t \in \mathbb{R}^+\}$ on $h_0 \otimes \mathbf{H}$ given by

$$U(t) = \hat{W}(t) V_A(t) \tag{5.6}$$

then since $dV_A(t) = iV_A(t)H_A\, dt$ we have

$$dU(t) = d\hat{W}(t) V_A(t) + iU(t)H_A\, dt.$$

Now $G(t) = V_A(t)G(0)V_A(t)^*$ whence we obtain

$$\begin{aligned} dU &= U[G(0)^* dA - G(0)dA^\dagger + (iH_A \\ &\quad - \tfrac{1}{2}\lambda^2 G^\dagger(0)^* G(0) - \tfrac{1}{2}\mu^2 G(0)G(0)^*)dt], \\ U(0) &= I. \end{aligned} \tag{5.7}$$

We obtain a slight simplification of (5.7) by writing $G(0) = iG$ and using the invariance of quantum Brownian motion under the gauge transformation $A \to e^{i\theta}A$ (Ref. 5), with $\theta = \pi/2$, to transform (5.7) to

$$dU = U[G^* dA - G\,dA^\dagger + (iH_A - \tfrac{1}{2}\lambda^2 G^* G - \tfrac{1}{2}\mu^2 GG^*)dt], \quad U(0) = I. \tag{5.8}$$

Thus we may substitute (5.6) into (3.5) to obtain a dilation of the quantum dynamical semigroup on $M_2(\mathbb{C})$ with generator

$$L(X) = i[H_A, X] + \lambda^2(G^* XG - \tfrac{1}{2}\{G^* G, X\}) + \mu^2(GXG^* - \tfrac{1}{2}\{GG^*, X\}), \tag{5.9}$$

where $X \in M_2(\mathbb{C})$.

We explicitly represent L as an element of $M_4(\mathbb{C})$ with respect to the basis $\{aa^\dagger, a^\dagger a, a, a^\dagger\}$ of $M_2(\mathbb{C})$ to obtain

$$\begin{pmatrix} -(\lambda^2\epsilon^2 + \eta^2\mu^2) & \lambda^2\eta^2 + \epsilon^2\mu^2 & 0 & 0 \\ \lambda^2\epsilon^2 + \eta^2\mu^2 & -(\lambda^2\eta^2 + \epsilon^3\mu^2) & 0 & 0 \\ 0 & 0 & -iw - \tfrac{1}{2}\sigma^2(\eta^2 + \epsilon^2) & \sigma^2\eta\epsilon \\ 0 & 0 & \sigma^2\eta\epsilon & iw - \tfrac{1}{2}\sigma^2(\eta^2 + \epsilon^2) \end{pmatrix} \tag{5.10}$$

(cf. Ref. 7).

Note that in the case $\eta = \epsilon = 0$ when there is no interaction, $U(t) = V_A(t)$ and (5.9) is simply the expression for the (reversible) dynamics on $M_2(\mathbb{C})$, in the Heisenberg picture, induced by $V_A(t)$.

The case $\epsilon = \eta = 1$, corresponding to the interaction Hamiltonian H_I^0, yields in (5.8)

$$dU = U(iqdP + (iH_A - \tfrac{1}{2}\sigma^2 q)dt), \quad U(0) = I, \tag{5.11}$$

where $q = a + a^*$ and $P(t) = -i(A(t) - A^\dagger(t))$ $(t \geqslant 0)$. Equation (5.11) has the explicit solution

$$U(t) = \exp(itH_A + iqP(t)). \tag{5.12}$$

We note that $P = (P(t),\ t \geqslant 0)$ is a realization of classical Brownian motion.[5]

Comparing the form of (5.8) with Sec. IV of Ref. 24, we find that the rotating wave approximation ($\epsilon = 0$) and antirotating wave approximation ($\eta = 0$) yield dilations of semigroups yielding two of the three standard forms of the Bloch equations.

VI. PROPERTIES OF THE REDUCED EVOLUTION

We now investigate to see if the dilation we have constructed is stationary with respect to the given initial state τ^0, where

$$\tau^0(X) = \operatorname{tr}\rho_A X \quad \text{for } X \in M_2(\mathbb{C})$$

and the state $\tilde{\tau} = \tau^0 \otimes \tau_\mu$. To do this we must verify the detailed balance condition (3.9).

Clearly $\rho_A^{it} H_A \rho_A^{-it} = H_A$ and we have

$$\rho_A^{it} G \rho_A^{-it} = \begin{pmatrix} e^{(1/2)it\beta w_0} & 0 \\ 0 & e^{-(1/2)it\beta w_0} \end{pmatrix} \begin{pmatrix} 0 & \eta \\ \epsilon & 0 \end{pmatrix} \times \begin{pmatrix} e^{-(1/2)it\beta w_0} & 0 \\ 0 & e^{(1/2)it\beta w_0} \end{pmatrix} = e^{it\beta w_0}\eta a + e^{-it\beta w_0}\epsilon a^*.$$

Thus we see that the detailed balance condition is satisfied (with $\alpha = \beta w_0$) only in the case $\epsilon = 0$ and we have proved the following.

Theorem 2: The stochastic Wigner–Weisskopf atom satisfies quantum detailed balance with respect to τ^0 if and only if the rotating wave approximation is made. It is only under this condition that the dilation is stationary with respect to τ^0 and $\tilde{\tau}$.

Since, in general, the state τ^0 is not left invariant by the action of the semigroup (5.9), we will compute its evolution. We obtain a positive, trace-preserving semigroup of linear operators $\{T_t^*,\ t \geqslant 0\}$ on $M_2(\mathbb{C})$ by the duality

$$\operatorname{tr}(XT_t(Y)) = \operatorname{tr}(T_t^*(X)Y) \tag{6.1}$$

for $X, Y \in M_2(\mathbb{C})$.

We aim to compute $\rho_t = T_t^*(\rho_A)$ for $t \geqslant 0$. From (5.10) we observe that

$$L(aa^\dagger) = -L(a^\dagger a),$$

whence we obtain

$$T_t(aa^*) = aa^* - (1/\Delta)(\psi aa^* - \chi a^* a)(1 - e^{-t\Delta}),$$
$$T_t(a^* a) = a^* a - (1/\Delta)(\chi a^* a - \psi aa^*)(1 - e^{-t\Delta}), \tag{6.2}$$

for $t \geqslant 0$, where

$$\chi = \lambda^2\eta^2 + \epsilon^2\mu^2, \quad \psi = \lambda^2\epsilon^2 + \eta^2\mu^2, \quad \Delta = \sigma^2(\eta^2 + \epsilon^2). \tag{6.3}$$

Now substituting (6.2) and (4.2) in (6.1) we find

$$\rho_t = \rho_A - (\epsilon^2/\Delta)(1 - e^{-t\Delta})(aa^* - a^* a) \tag{6.4}$$

for $t \geqslant 0$.

For nonzero G we find from (6.4) that $\rho_t = \rho_A$ (for all $t > 0$) if and only if $\epsilon = 0$, as we expect from Theorem 2.

In the general case, the system tends to a new equilibrium state ρ_∞, where

$$\rho_\infty = \rho_A - (\epsilon^2/\Delta)(aa^* - a^* a). \tag{6.5}$$

For each $t \geqslant 0$, we write the Gibbs density matrix ρ_t in the form

$$e^{-\beta(t)H_A}/\operatorname{tr}(e^{-\beta(t)}H_A),$$

where $\beta(t)$ is a time dependent inverse temperature. From (6.3) and (6.4) we obtain

$$\beta(t) = \beta + \tilde{\beta}(t),$$

where

$$\tilde{\beta}(t) = \frac{1}{w_0} \ln\left[\frac{1 - k(t)(1 - e^{-\beta w_0})}{1 + k(t)(e^{\beta w_0} - 1)}\right] \tag{6.6}$$

and

$$k(t) = [\epsilon^2/(\epsilon^2 + \eta^2)](1 - e^{-t\Delta}), \quad t \geqslant 0. \tag{6.7}$$

It is easily verified from (6.6) that $\beta(t)$ decreases monotonically to β_∞, where

$$\rho_\infty = e^{-\beta_\infty H_A}/\mathrm{tr}(e^{-\beta_\infty H_A})$$

and

$$\beta_\infty = \beta - \frac{1}{w_0} \ln\left(\frac{\eta^2 + \epsilon^2}{\eta^2 + \epsilon^2} \frac{e^{\beta w_0}}{e^{-\beta w_0}}\right).$$

We remark that the states we have considered are not the only ones for which the given dilation is stationary. For example, if we put $\epsilon = \eta$ and replace τ^0 by the normalized trace we obtain a stationary "essentially commutative" dilation[25] by reinterpreting (5.12) as a SDE in Wiener space and considering the restriction of $\frac{1}{2}\,\mathrm{tr} \otimes \tau_0$ to $M_2(\mathbb{C})$ tensored with the L^∞ space of Wiener measure. The detailed balance condition is also satisfied for this case. However this dilation could not be constructed by our technique since to obtain the normalized trace as an initial state we must take $\alpha = 0$, whence λ and μ are undefined.

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Relativistic charged bosons in a magnetic field. I. Wave functions and matrix elements

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A system of charged zero-spin bosons in the presence of a uniform magnetic field is studied using a relativistic spinor formalism. Equations of motion for the relevant operators are developed. The eigenfunctions of two different sets of commuting operators are obtained by the use of ladder operators and also by direct solution of the Klein–Gordon equation in both coordinate and momentum representations. Matrix elements are calculated which will be required in later consideration of the collisionless conductivity and dielectric tensors for the boson–antiboson plasma in a strong magnetic field (see papers II and III in this series).

I. INTRODUCTION

The charged zero-spin Bose gas has been extensively investigated in the nonrelativistic domain for its intrinsic interest as a many-body system. Hore and Frankel[1] have given a literature review of the older nonrelativistic material that originated with Foldy.[2]

Intensive study over recent years of the relativistic fermion plasma (Kowalenko, Frankel, and Hines[3–5] and references therein) provided the techniques used later for an extension of the boson work into the relativistic domain also. This enables an instructive comparison between the boson and the fermion work to be made and highlights for both the plasma and the vacuum properties of such systems the intrinsic behavior that arises from the fundamental particle statistics. Any practical application of this work would treat charged pions in astrophysical situations where ultrastrong magnetic fields exist.

The work of Hines and Frankel[6] initiated the study of the relativistic charged Bose gas, but antibosons were omitted from consideration as the investigations were confined to the region below pair threshold. The generalization of the dielectric response function method to a relativistic charged Bose plasma above pair threshold has been published in three papers by Kowalenko, Frankel, and Hines.[3–5] In these calculations the $T = 0$ K ground state properties of the system are investigated and antibosons have been included but, in contrast to the fermion work, there is a restriction to zero magnetic field.

In the work detailed by Kowalenko, Frankel, and Hines,[3–5] the second quantized Hamiltonian for a plasma of charged bosons and antibosons has been used in the two-component spinor representation to provide linearized equations of motion for the four generalized distribution functions pertaining, respectively, to bosons, antibosons, and mixtures of the two. Fourier–Laplace transformation of the equations of evolution for these distribution functions, together with Poisson's equation, leads to the expression for the frequency- and wave-number-dependent longitudinal dielectric response function.

This work requires extension in several ways. These involve the inclusion of a magnetic field, the calculation of the full repsonse tensor instead of just the longitudinal response, and finally the removal of the limitation to zero temperature. For a boson–antiboson plasma in an external magnetic field and at arbitrary temperature the general form of the conductivity tensor $\tilde{\sigma}$ will be developed in the second paper of the present series[7] (hereafter referred to as Paper II). In the present paper we evaluate the matrix elements occurring in the general result for $\tilde{\sigma}$ and will thus be in a position to reduce and simplify the full response tensor in Paper II. In order to include the effects due to an external, intense magnetic field in calculating the full response tensor, it is necessary to use wave functions appropriate to bosons and antibosons in the presence of such a field. The calculation of the wave functions in the case of fermions is straightforward and is given, for example, in the well-known paper by Johnson and Lippmann.[8] For bosons, however, so far as the authors are aware, there is no comparable calculation.

To begin with, therefore, we present a comprehensive treatment of the Klein–Gordon equation in the presence of an external magnetic field and calculate all the matrix elements required for the response tensor. Section II defines the spinor formalism and the conventions used. In general we follow the method of Johnson and Lippmann, adapted for bosons. The Heisenberg equations of motion for the relevant operators are studied in Sec. III. In Sec. IV the calculation of the eigenfunctions is presented in two different ways: first, using ladder operators to generate them from the ground state eigenfunction and, alternatively, from the direct solution of the Klein–Gordon equation. In this latter treatment two different sets of eigenvectors are employed: one set that contains eigenvectors of the z component of angular momentum (L_z) and the other set eigenvectors of the x component of the canonical momentum (p_x), for which the development is particularly simple and has been studied previously by Rapaport.[9] Both of these forms of the solution are used to calculate some significant expectation values, including those of the momentum and position operators. The eigenfunctions of p_x in a momentum representation are included for completeness.

In Sec. V we calculate the matrix elements that will be required in Paper II for a discussion of the full response

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tensor for the boson–antiboson system in a magnetic field. It emerges that the matrix elements required are of three basic forms:

$$\langle \epsilon',p'|e^{iq\cdot r}|\epsilon,p\rangle = \int \Psi^{\dagger}_{\epsilon',p'}(\mathbf{r},t)\tau_3 e^{iq\cdot r}\Psi_{\epsilon,p}(\mathbf{r},t)d^3r, \tag{1a}$$

$$\langle \epsilon',p'|\tau_0 e^{iq\cdot r}|\epsilon,p\rangle = \int \Psi^{\dagger}_{\epsilon',p'}(\mathbf{r},t)\tau_3\tau_0 e^{iq\cdot r}\Psi_{\epsilon,p}(\mathbf{r},t)d^3r, \tag{1b}$$

and

$$\langle \epsilon',p'|\tau_0 e^{iq\cdot r}\boldsymbol{\pi}|\epsilon,p\rangle = \int \Psi^{\dagger}_{\epsilon',p'}(\mathbf{r},t)\tau_3\tau_0 e^{iq\cdot r}\boldsymbol{\pi}\Psi_{\epsilon,p}(\mathbf{r},t)d^3r, \tag{1c}$$

where $\epsilon, \epsilon' = +1$ or -1 and the wave functions $\Psi_{+,p}(\mathbf{r},t)$ and $\Psi_{-,p}(\mathbf{r},t)$ represent the positive and negative energy solutions, respectively, of the Klein–Gordon equation in the spinor representation. The 2×2 matrices τ_0 and τ_3 are defined in Sec. II and $\boldsymbol{\pi}$ is the kinetic momentum.

SI units are used throughout our calculations. The charge on the boson is $+e$.

II. SPINOR FORMALISM

The scalar wave function ψ for zero-spin bosons is the solution of the Klein–Gordon equation:

$$[(\mathbf{p}-e\mathbf{A})^2 + m^2c^2]\psi = E^2\psi/c^2. \tag{2}$$

The kinetic momentum $\boldsymbol{\pi}$ is related to the canonical momentum $\mathbf{p}$ by $\boldsymbol{\pi} = \mathbf{p} - e\mathbf{A}$ and satisfies the commutation relations

$$(\boldsymbol{\pi}\times\boldsymbol{\pi}) = ie\hbar\mathbf{B}. \tag{3}$$

A Hamiltonian formulation of the problem is developed with a 2×2 spinor operator following the approach of Davydov[10] and Feshbach and Villars.[11] We therefore write

$$H = (1/2m)(\tau_3 + i\tau_2)\boldsymbol{\pi}^2 + mc^2\tau_3, \tag{4}$$

where the τ's are 2×2 matrices defined as follows:

$$\tau_1 = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \quad \tau_2 = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix},$$
$$\tau_3 = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}, \quad \tau_0 = \tau_3 + i\tau_2. \tag{5}$$

The τ_i $(i = 1,2,3)$ satisfy the relations

$$\tau_j\tau_k = -\tau_k\tau_j = i\epsilon_{jkl}\tau_l, \quad j\neq k$$

and

$$\tau_i^2 = I = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}.$$

The spinor wave functions in this Hamiltonian formulation are expressed in terms of two-component column vectors such that

$$\Psi = \begin{pmatrix}\xi\\ \chi\end{pmatrix}, \tag{6}$$

where ξ and χ are related to ψ by the equations

$$\psi = \xi + \chi \tag{7a}$$

and

$$i\hbar\frac{\partial\psi}{\partial t} - e\phi\psi = mc^2(\xi - \chi). \tag{7b}$$

Here ϕ is the electrostatic potential. For the stationary case in a uniform magnetic field with energy eigenvalue E, the relationship between the spinor components and the scalar wave function simplifies to

$$\xi = (1/2mc^2)(mc^2 + E)\psi \tag{8a}$$

and

$$\chi = (1/2mc^2)(mc^2 - E)\psi. \tag{8b}$$

The appropriate normalization in a coordinate representation is to make the charge density plus or minus unity, i.e.,

$$\int \Psi^{\dagger}_{\alpha}(\mathbf{r})\tau_3\Psi_{\alpha}(\mathbf{r})d^3r = \pm 1. \tag{9}$$

Expectation values of an operator O are given by

$$\langle\alpha|O|\beta\rangle = \int \Psi^{\dagger}_{\alpha}(\mathbf{r})\tau_3 O\Psi_{\beta}(\mathbf{r})d^3r \tag{10}$$

in a coordinate representation and in a momentum representation by

$$\langle\alpha|O|\beta\rangle = \int \Psi^{\dagger}_{\alpha}(\mathbf{p})\tau_3 O\Psi_{\beta}(\mathbf{p})d^3p. \tag{11}$$

Correspondingly, the completeness relation departs from the usual form because of the inclusion of the τ_3 matrix:

$$\sum_{\gamma}\Psi^{\dagger}_{\gamma}(\mathbf{r}')\tau_3\Psi_{\gamma}(\mathbf{r}) = \delta^3(\mathbf{r}'-\mathbf{r}). \tag{12}$$

As a consequence, expansions of $\langle\alpha|O_1O_2|\beta\rangle$ in terms of matrix elements of O_1 and O_2 do not take the usual form. That is,

$$\langle\alpha|O_1O_2|\beta\rangle \neq \sum_{\gamma}\langle\alpha|O_1|\gamma\rangle\langle\gamma|O_2|\beta\rangle.$$

An example of such an expansion is given in Sec. V.

The τ_3 matrix modifies the standard definition of the adjoint operator $O^{\ddagger}$ to O, so that

$$\langle\alpha|O|\beta\rangle = \langle\beta|O^{\ddagger}|\alpha\rangle^* \tag{13}$$

with $O^{\ddagger} = \tau_3 O^{\dagger}\tau_3$.

III. EQUATIONS OF MOTION

The equation of motion of an operator X in the Heisenberg picture is

$$i\hbar\dot{X} = [X,H]. \tag{14}$$

Following Johnson and Lippmann,[8] the evolution of the kinetic momentum components is given by

$$\dot{\pi}_x = \omega_c\tau_0\pi_y, \tag{15a}$$

$$\dot{\pi}_y = -\omega_c\tau_0\pi_x, \tag{15b}$$

and

$$\dot{\pi}_z = 0, \tag{15c}$$

where $\omega_c = eB/m$ and the magnetic field is aligned in the z direction. For the position operator $\mathbf{r}$,

$$m\dot{\mathbf{r}} = \tau_0\boldsymbol{\pi}. \tag{16}$$

From Eq. (15c) it is obvious that the momentum along the z axis, i.e., parallel to $\mathbf{B}$, is constant.

Further constants of the motion are obtained by eliminating π_x and π_y between Eqs. (15) and (16):

$$\frac{d}{dt}(\pi_x - m\omega_c y) = 0, \tag{17a}$$

$$\frac{d}{dt}(\pi_y + m\omega_c x) = 0. \tag{17b}$$

These equations lead upon integration to two constants, the x and y coordinates of the center of gyration, x_0 and y_0:

$$y_0 = y - \pi_x/m\omega_c, \tag{18a}$$

$$x_0 = x + \pi_y/m\omega_c. \tag{18b}$$

Classically the coordinates of the guiding center are given by $x_0 = x + v_y/\omega_c$ and $y_0 = y - v_x/\omega_c$. The integration constants x_0 and y_0 commute with H, π_x, and π_y but not with each other, as

$$[x_0, y_0] = -i\hbar/eB = -i\lambda^2. \tag{19}$$

Here λ is a fundamental quantum scale length for any particle in a magnetic field of this magnitude.

A simple combination of x_0 and y_0 in the form $r_0^2 = x_0^2 + y_0^2$ is obviously constant and the square of the radius of gyration r_1 defined by

$$r_1^2 = (x - x_0)^2 + (y - y_0)^2 \tag{20}$$

is also an invariant. This is easily seen by substituting Eq. (18) into (20) to obtain

$$r_1^2 = (1/m^2\omega_c^2)(\pi_x^2 + \pi_y^2) = \pi_\perp^2/m^2\omega_c^2 \tag{21}$$

and by noting that $\pi_\perp^2$ is conserved, since $[\pi_\perp^2, H] = 0$. This is identical to the classical result, where $r_1^2 = (1/\omega_c^2)(v_x^2 + v_y^2)$ is conserved.

If a symmetric gauge is used, so that $\mathbf{A} = \frac{1}{2}\mathbf{B}\times\mathbf{r}$, then the angular momentum about the z axis, L_z, is given by

$$L_z = (\mathbf{r}\times\mathbf{p})_z$$
$$= x\pi_y - y\pi_x + m\omega_c/2(x^2 + y^2). \tag{22}$$

By using the equations of motion for $\mathbf{r}$ and $\boldsymbol{\pi}$, i.e., Eqs. (15) and (16), it can be shown that $\dot{L}_z = 0$ and so L_z is also a constant of the motion, again identical with the classical result. Alternatively, L_z can be expressed in terms of r_0 and r_1 using Eqs. (18) and (21):

$$L_z = m\omega_c[-x(x - x_0) - y(y - y_0) + \tfrac{1}{2}(x^2 + y^2)]$$
$$= (m\omega_c/2)(r_0^2 - r_1^2). \tag{23}$$

While r_0 and r_1 are precisely known, there is an uncertainty in locating points on the boson's orbit as the commutation relation between x_0 and y_0, Eq. (19), implies that $\Delta x_0 \Delta y_0 \geq \frac{1}{2}\lambda^2$. This prevents us from knowing the exact location of the orbit's guiding center.

In the Heisenberg picture the τ's also have equations of motion which can be obtained using Eq. (14) and the relations

$$\{\tau_1, H\} = 0, \tag{24a}$$

$$\{\tau_2, H\} = i\pi^2 I/m, \tag{24b}$$

$$\{\tau_3, H\} = \pi^2 I/m + 2mc^2 I, \tag{24c}$$

$$[\tau_2, H] = (i/mc^2)(H^2 + m^2c^4)\tau_1, \tag{24d}$$

$$[\tau_3, H] = \pi^2\tau_1/m. \tag{24e}$$

The equations of motion for the τ's therefore become

$$\dot{\tau}_1 = (i/m\hbar)(\tau_3 + i\tau_2)\pi^2 - 2mc^2\tau_2/\hbar, \tag{25a}$$

$$\dot{\tau}_2 = \pi^2\tau_1/m\hbar + 2mc^2\tau_1/\hbar, \tag{25b}$$

$$\dot{\tau}_3 = -i\pi^2\tau_1/m\hbar. \tag{25c}$$

Since $\tau_i(t) = \exp\{iHt/\hbar\}\tau_i(0)\exp\{-iHt/\hbar\}$, the solutions of Eq. (25) for the τ's are

$$\tau_1(t) = \exp\{2iHt/\hbar\}\tau_1(0), \tag{26a}$$

$$\tau_2(t) = \exp\{2iHt/\hbar\}\tau_2(0) + (I\pi^2/m) \times\exp\{iHt/\hbar\} f(t), \tag{26b}$$

and

$$\tau_3(t) = \tau_3(0) - (i\pi^2/m) \times\exp\{iHt/\hbar\} f(t)\tau_1(0), \tag{26c}$$

where the $\tau(0)$'s are given by Eq. (5) and

$$f(t) = \sum_{k=0}^{\infty} \frac{(-1)^k (t/\hbar)^{2k+1} H^{2k}}{(2k+1)!}. \tag{27}$$

Note that $f(t)$ has the properties

$$Hf(t) = \sin(Ht/\hbar) \tag{28a}$$

and

$$\frac{df(t)}{dt} = \frac{1}{\hbar}\cos\left(\frac{Ht}{\hbar}\right). \tag{28b}$$

From the definition of H we obtain the expected result that

$$H^2 = \pi^2c^2 + m^2c^4. \tag{29}$$

Separating π^2 into its transverse and parallel components recasts H^2 into the form

$$H^2 = 2mc^2H_\perp + \pi_z^2c^2 + m^2c^4, \tag{30}$$

where

$$H_\perp = (1/2m)(\pi_x^2 + \pi_y^2). \tag{31}$$

Since $H_\perp$ commutes with H, these operators share an identical complete set of eigenvectors. Equation (31), together with the commutation relations between π_x and π_y, i.e., Eq. (3), now define an eigenvalue problem identical to that for the two-dimensional harmonic oscillator. Hence the eigenvalues of $H_\perp$ are $\hbar\omega_c(\nu + \frac{1}{2})$ with $\nu = 0,1,2,3,\ldots$. As the eigenvalue of π_z is p_z, the square of the energy eigenvalue, E_ν, is given by

$$E_\nu^2 = 2mc^2[\hbar\omega_c(\nu + \tfrac{1}{2})] + p_z^2c^2 + m^2c^4$$
$$= |e|B\hbar c^2(2\nu + 1) + p_z^2c^2 + m^2c^4. \tag{32}$$

In relativistic quantum mechanics certain operators, such as the "velocity" operator $\dot{\mathbf{r}}$, can no longer be interpreted as single particle operators. This is because the complete space of eigenfunctions has two subspaces of positive and negative energy eigenfunctions. It is those operators, called even operators, which do not mix these charge states that can still be given a single particle interpretation. Some examples of these even operators are τ_3, $\boldsymbol{\pi}$, and H. Conversely, an odd operator is one that maps eigenfunctions of one charge

state into the other. Now, any operator can be expressed as the sum of even and odd operators and so it is useful to study the even components. In a similar way to the Feshbach–Villars transformation,[10,11] we seek a generalized transformation which maps the spinor eigenfunctions into $\binom{1}{0}$ or $\binom{0}{1}$ column spinors depending on whether they are positive or negative eigenfunctions. This generalized transformation leads to the Φ representation where the independent variable is $\mathbf{p}$ and in which even operators are diagonal 2×2 matrices and odd operators are off-diagonal 2×2 matrices. The transformation is

$$\Phi(\mathbf{p}) = V\Psi(\mathbf{p}),$$

where

$$V = [I(E+mc^2) + \tau_1(E-mc^2)]/2\sqrt{mc^2E}, \tag{33}$$

while $\Phi^\dagger = \Psi^\dagger V^{-1}$ with

$$V^{-1} = \tau_3 V \tau_3 = [I(E+mc^2) - \tau_1(E-mc^2)]/2\sqrt{mc^2E}. \tag{34}$$

Here $E = E(p_z,\nu)$ is the energy eigenvalue corresponding to the state $\Phi(\mathbf{p})$. The new Hamiltonian H_Φ is given by

$$H_\Phi = VHV^{-1} = (1/2E)[(\tau_3 + i\tau_2)\pi^2c^2 + \tau_3(E^2 + m^2c^4) - i\tau_2(E^2 - m^2c^4)] \tag{35}$$

and since $\pi^2c^2 = E^2 - m^2c^4$, when H_Φ acts on Φ we obtain

$$H_\Phi\Phi = \tau_3 E\Phi. \tag{36}$$

As τ_3 is even, H_Φ is also even, as expected. However, the coordinate operator $\mathbf{r} = i\hbar\nabla_p$ is transformed into

$$\mathbf{r}_\Phi = V(i\hbar\nabla_p)V^{-1} = i\hbar\nabla_p - i\hbar p_z c^2\tau_1\hat{k}/2E^2, \tag{37}$$

which has an even component, $[\mathbf{r}_\Phi] = i\hbar\nabla_p$, and an odd component $\{\mathbf{r}_\Phi\} = -i\hbar p_z c^2\tau_1\hat{k}/2E^2$. Here $\hat{k}$ is the unit vector in the direction of $\mathbf{B}$. Using Eq. (14) gives

$$\frac{d}{dt}[\mathbf{r}_\Phi] = \frac{p_z c^2\tau_3\hat{k}}{E}. \tag{38}$$

The left-hand side of Eq. (38) represents the average velocity operator and, as required, has only a component parallel to the magnetic field.

IV. EIGENFUNCTIONS

The eigenfunctions of our system are eigenfunctions of the Hamiltonian H and $\pi_z = p_z$, but these two alone are insufficient to resolve the infinite degeneracy which appears. Another operator, which commutes with these two, is needed to determine the eigenvalue problem completely. Any function of the coordinates of the guiding center, x_0 and y_0, is such an operator. So the form of the set of eigenfunctions will depend on the choice for the third operator. There are three simple and conventional choices x_0, y_0, and r_0^2.

In the case of x_0 the guiding center is located in the plane $x = x_0$ and the y_0 coordinate is undefined. If the gauge $\mathbf{A} = \hat{j}Bx$ is used this choice is equivalent to choosing $p_y = eBx_0$ as the third operator.

If we choose y_0 the guiding center is located in the plane $y = y_0$ and using the gauge $\mathbf{A} = -\hat{i}By$ makes this choice equivalent to that of $p_x = -eBy_0$.

If r_0^2 is used the guiding center is localized on a cylindrical shell of radius $\lambda(2s+1)^{1/2}$, where $s = 0,1,2,\ldots$. If the symmetric gauge $\mathbf{A} = \frac{1}{2}\mathbf{B}\times\mathbf{r}$ is used, this choice is equivalent to picking $L_z = \frac{1}{2}m\omega_c(r_0^2 - r_1^2)$ as the third operator with eigenvalues $\hbar(s-n) = l\hbar$, so $s = l+n$.

In addition to the choice of commuting operators there are two ways to calculate the eigenfunctions. The first is to continue with the harmonic oscillator analogy mentioned in Sec. III to find the ground state ψ_0 and build up the eigenfunctions using ladder operators $\pi_\pm = \pi_x \mp i\pi_y$ (see Sec. IV A). Another way is to solve the Klein–Gordon equation directly for ψ (see Secs. IV B–IV D).

A. Ladder operators applied to eigenfunctions of $\{H,\pi_z,y_0\}$

We use an asymmetric gauge $A = -B\hat{y}\hat{i}$. Hence

$$\pi_\pm = -i\hbar\frac{\partial}{\partial x} + eBy \mp \hbar\frac{\partial}{\partial y}. \tag{39}$$

If ψ_ν is a scalar eigenfunction of H^2 or $H_\perp$, with a level number ν, then $\pi_+\psi_\nu$ and $\pi_-\psi_\nu$ are eigenfunctions with level numbers $\nu+1$ and $\nu-1$, respectively. Therefore the defining equations for the ground state ψ_0 are

$$\pi_-\psi_0 = 0, \tag{40}$$

$$\pi_z\psi_0 = p_z\psi_0, \tag{41a}$$

and

$$\hat{p}_x\psi_0 = p_x\psi_0. \tag{41b}$$

Solving for ψ_0 yields

$$\psi_0 = K_0\exp\left\{\frac{i}{\hbar}(xp_x + zp_z) - \frac{1}{2\lambda^2}\left(y + \frac{p_x}{eB}\right)^2\right\}, \tag{42}$$

where K_0 is the normalization constant for $\nu = 0$ and p_x and p_z are eigenvalues of $\hat{p}_x$ and π_z, respectively. The general wave function ψ_ν is expressed in terms of

$$\psi_\nu = K_\nu\exp\left\{\frac{i}{\hbar}(xp_x + zp_z) - \frac{1}{2\lambda^2}\left(y + \frac{p_x}{eB}\right)^2\right\} f_\nu(y). \tag{43}$$

By acting upon the exponential term in Eq. (42) with π_+ repeatedly it can be shown that

$$f_\nu(y) = H_\nu[(1/\lambda)(y + (p_x/eB))], \tag{44}$$

where H_ν is a Hermite polynomial. Normalization yields the explicit wave function

$$\psi_\nu(x,y,z) = \left[\frac{mc^2}{\sqrt{\pi}\lambda\mathscr{L}_x\mathscr{L}_z 2^\nu\nu!E_\nu}\right]^{1/2} H_\nu\left(\frac{1}{\lambda}\left(y + \frac{p_x}{eB}\right)\right) \times\exp\left\{\frac{i}{\hbar}(xp_x + zp_z) - \frac{1}{2\lambda^2}\left(y + \frac{p_x}{eB}\right)^2\right\}, \tag{45}$$

where $\mathscr{L}_x$ and $\mathscr{L}_z$ are lengths of the system in the x and z directions, respectively. In terms of the ground state we have

$$\psi_\nu = \left(\frac{E_0}{2^\nu \nu! E_\nu}\right)^{1/2} \left(\frac{\lambda \pi_+}{\hbar}\right)^\nu \psi_0, \tag{46}$$

while $\psi_{\nu+1}$ and $\psi_{\nu-1}$ are related to ψ_ν by

$$\psi_{\nu+1} = \left(\frac{E_\nu}{2(\nu+1)E_{\nu+1}}\right)^{1/2} \frac{\lambda \pi_+}{\hbar} \psi_\nu \tag{47a}$$

and

$$\psi_{\nu-1} = \left(\frac{E_\nu}{2\nu E_{\nu-1}}\right)^{1/2} \frac{\lambda \pi_-}{\hbar} \psi_\nu. \tag{47b}$$

B. Solution of the Klein–Gordon equation for eigenfunctions of $\{H,\pi_z,y_0\}$ in a coordinate representation

We now give an alternative derivation of ψ_ν and E_ν. Using $\mathbf{A} = -By\hat{i}$, the Klein–Gordon equation becomes

$$[(p_y^2 + p_z^2)c^2 + (p_x + eBy)^2 c^2 + m^2c^4 - E^2]\psi = 0. \tag{48}$$

As x and z are cyclic coordinates, the solution is of the form given by Rapaport[9]:

$$\psi_{p_x p_z}(\mathbf{r}) = \exp\{(i/\hbar)(xp_x + zp_z)\}\phi(y). \tag{49}$$

Making the transformation

$$\xi = (y - y_0)/\lambda \tag{50}$$

results in

$$\frac{d^2\phi(\xi)}{d\xi^2} + \left(\frac{E^2 - m^2c^4 - p_z^2c^2}{|e|B\hbar c^2} - \xi^2\right)\phi(\xi) = 0, \tag{51}$$

which has the solution

$$\phi(\xi) = \text{const} \times \exp\{-\tfrac{1}{2}\xi^2\} H_\nu(\xi) \tag{52}$$

with the condition that

$$(E^2 - m^2c^4 - p_z^2c^2)/|e|B\hbar c^2 = 2\nu + 1, \tag{53}$$

where $\nu = 0,1,2,\ldots$. Normalizing according to Eq. (9) yields

$$\psi_{p_x p_z \nu}(x,y,z) = \left[\frac{mc^2}{\sqrt{\pi}\lambda \mathscr{L}_x \mathscr{L}_z E_\nu 2^\nu \nu!}\right]^{1/2} \times \exp\left\{\frac{i}{\hbar}(xp_x + zp_z) - \frac{1}{2\lambda^2}(y - y_0)^2\right\} \times H_\nu\left[\frac{1}{\lambda}(y - y_0)\right],$$

while Eq. (53) leads to

$$E_\nu^2 = m^2c^4 + p_z^2c^2 + eB\hbar c^2(2\nu + 1).$$

These results are identical to the earlier ones.

From Eqs. (6) and (8) the boson spinor wave function now becomes

$$\Psi_{+,p}(\mathbf{r},t) = \frac{1}{\sqrt{\lambda \mathscr{L}_x \mathscr{L}_z}} \begin{pmatrix} \sqrt{mc^2/E_\nu} + \sqrt{E_\nu/mc^2} \\ \sqrt{mc^2/E_\nu} - \sqrt{E_\nu/mc^2} \end{pmatrix} \times \frac{1}{\sqrt{\pi^{1/2} 2^{\nu+2} \nu!}} \times H_\nu\left[\frac{1}{\lambda}(y - y_0)\right] \times \exp\left\{-\frac{iE_\nu t}{\hbar} + \frac{i}{\hbar}(xp_x + zp_z) - \frac{1}{2\lambda^2}(y - y_0)^2\right\}, \tag{54}$$

where p is the set of quantum numbers $\{p_x,p_z,\nu\}$. The antiboson wave function is found simply by reversing the signs of all momenta and energy eigenvalues E_ν, p_x, and p_z (this operation performed on the Klein–Gordon equation is equivalent to reversing the sign of the charge e). The antiboson spinor wave function is then

$$\Psi_{-,p}(\mathbf{r},t) = \frac{1}{\sqrt{\lambda \mathscr{L}_x \mathscr{L}_z}} \begin{pmatrix} \sqrt{mc^2/E_\nu} - \sqrt{E_\nu/mc^2} \\ \sqrt{mc^2/E_\nu} + \sqrt{E_\nu/mc^2} \end{pmatrix} \times \frac{1}{\sqrt{\pi^{1/2} 2^{\nu+2} \nu!}} H_\nu\left[\frac{1}{\lambda}(y + y_0)\right] \times \exp\left\{\frac{iE_\nu t}{\hbar} - \frac{i}{\hbar}(xp_x + zp_z) - \frac{1}{2\lambda^2}(y + y_0)^2\right\}. \tag{55}$$

These two sets of eigenfunctions form a complete orthonormal basis for the Hilbert space

$$\langle \epsilon',p' | \epsilon,p \rangle = \epsilon \delta_{\epsilon,\epsilon'} \delta_{p,p'}. \tag{56}$$

It should be noted that the charge conjugate spinor function, $\Psi^c \equiv \tau_1 \Psi^\dagger = (\chi^* \; \xi^*)$, where $\Psi^\dagger = \begin{pmatrix} \xi^* \\ \chi^* \end{pmatrix}$ is not the antiparticle state in an electromagnetic field.

Furthermore, if the spinor wave function is written in the form

$$\Psi_{\epsilon,p}(\mathbf{r}) = \left(\frac{1}{\lambda \mathscr{L}_x \mathscr{L}_z}\right)^{1/2} \times \begin{pmatrix} \sqrt{mc^2/E_p} + \epsilon\sqrt{E_p/mc^2} \\ \sqrt{mc^2/E_p} - \epsilon\sqrt{E_p/mc^2} \end{pmatrix} \varphi_{\epsilon,p}(\mathbf{r}), \tag{57}$$

then the completeness relation becomes

$$\lambda \mathscr{L}_x \mathscr{L}_z \delta^3(\mathbf{r}' - \mathbf{r}) = \sum_\gamma \epsilon_\gamma \varphi_\gamma^*(\mathbf{r}') \varphi_\gamma(\mathbf{r}). \tag{58}$$

C. Solution of the Klein–Gordon equation for eigenfunctions of $\{H,\pi_z,y_0\}$ in a momentum representation

The procedure for determining the wave function in the momentum representation, $\psi(\mathbf{p})$, is formally similar to the case of the coordinate representation. The transformation of $y \to i\hbar(\partial/\partial y)$ is made in the Klein–Gordon equation, Eq. (48), so that the separation of momentum coordinates in the wave functions is clearly of the form

$$\psi_{p'_x p'_z}(\mathbf{p}) = \delta(p_x - p'_x)\delta(p_z - p'_z)\eta(p_y), \tag{59}$$

where p'_x and p'_z are the eigenvalues. The differential equation obtained is identical to Eq. (51) but with the dimensionless variable $\lambda p_y/\hbar$.

Solving the differential equation and normalizing yields

$$\psi_{p'_x,p'_z,\nu}(\mathbf{p}) = \left[\frac{\lambda mc^2}{\hbar\sqrt{\pi}2^\nu E_\nu \nu!}\right]^{1/2} \delta(p_x - p'_x)\delta(p_z - p'_z) \times \exp\left\{\frac{\lambda^2}{\hbar^2}\left(ip'_x p_y - \frac{1}{2}p_y^2\right)\right\} H_\nu\left[\frac{\lambda p_y}{\hbar}\right]. \tag{60}$$

Some interesting expectation values are readily calculated with eigenfunctions from Secs. IV A–IV C substituted into Eq. (10):

$$\langle y\rangle = \langle y_0\rangle = -(1/eB)\langle p_x\rangle, \tag{61}$$

$$\langle p_y\rangle = 0, \tag{62}$$

$$\langle \pi_x^2 + \pi_y^2\rangle = eB\hbar(2\nu + 1), \tag{63}$$

$$\langle r_1^2\rangle = \lambda^2(2\nu + 1). \tag{64}$$

D. Solution of the Klein–Gordon equation for eigenfunctions of $\{H,\pi_z,r_0^2\}$ in a coordinate representation

Here we use cylindrical polar coordinates (r,ϕ,z) and a symmetric gauge $\mathbf{A} = \frac{1}{2}(\mathbf{B}\times\mathbf{r})$ so that the following operator relations hold:

$$e^2B^2r_0^2 = \tfrac{1}{4}e^2B^2r^2 + p_\perp^2 + eBL_z, \tag{65}$$

$$\pi_\perp^2 = e^2B^2r_1^2 = p_\perp^2 - eBL_z + \tfrac{1}{4}e^2B^2r^2. \tag{66}$$

The corresponding classical expression is

$$m^2\gamma^2 v_\perp^2 = p_\perp^2 - eBL_z + \tfrac{1}{4}e^2B^2r^2. \tag{67}$$

The Klein–Gordon equation now becomes

$$\left\{\begin{array}{l} -\hbar^2c^2\left(\dfrac{\partial^2}{\partial r^2} + \dfrac{1}{r}\dfrac{\partial}{\partial r} + \dfrac{1}{r^2}\dfrac{\partial^2}{\partial\phi^2}\right) \\ +\tfrac{1}{4}e^2B^2c^2r^2 + m^2c^4 + p_z^2c^2 \\ -|e|B\hbar c^2|\ell| - E^2 \end{array}\right\}\psi(r,\phi,z) = 0, \tag{68}$$

where ℓ is the angular momentum quantum number and can take any integer value. As ϕ and z are cyclic coordinates in the Hamiltonian we take a trial solution of this equation of the form

$$\psi_{\ell,p_z}(\mathbf{r}) = \exp\{i\ell\phi + izp_z/\hbar\}f(r). \tag{69}$$

Equation (68) now becomes

$$\frac{d^2f(r)}{dr^2} + \frac{1}{r}\frac{df(r)}{dr} + \left(k - \frac{\ell^2}{r^2} - \frac{e^2B^2r^2}{4\hbar^2}\right)f(r) = 0, \tag{70}$$

where

$$k = (E^2 - m^2c^4 - p_z^2c^2 + |e|B\hbar c^2|\ell|)/\hbar^2c^2. \tag{71}$$

The nontrivial solution of Eq. (70) is

$$f(r) = \left(\frac{r^2}{2\lambda^2}\right)^{|\ell|/2}\exp\left\{-\frac{r^2}{4\lambda^2}\right\}L_n^{|\ell|}\left(\frac{r^2}{2\lambda^2}\right) \tag{72}$$

with the condition that

$$k = (|e|B/\hbar)(2n + |\ell| + 1). \tag{73}$$

Here $L_n^{|\ell|}(r^2/2\lambda^2)$ is a generalized Laguerre polynomial with $n = 0,1,2,3,\ldots$. Normalization results in

$$\psi_{n,\ell,p_z}(\mathbf{r}) = \left[\frac{mc^2n!}{2\pi\lambda^2\mathscr{L}_z E_n(n + |\ell|)!}\right]^{1/2} \times\left(\frac{r^2}{2\lambda^2}\right)^{|\ell|/2}L_n^{|\ell|}\left(\frac{r^2}{2\lambda^2}\right) \times\exp\{i\ell\phi + izp_z/\hbar - r^2/4\lambda^2\}, \tag{74}$$

while comparing Eqs. (71) and (73) shows that

$$E_n^2 = m^2c^4 + p_z^2c^2 + |e|B\hbar c^2(2n + 1). \tag{75}$$

Some expectation values calculated from these eigenfunctions are

$$\langle r_{n,|\ell|}^2\rangle = 2\lambda^2(2n + 1 + |\ell|), \tag{76}$$

$$\langle \pi_{\perp_n}^2\rangle = eB\hbar(2n + 1), \tag{77}$$

$$\langle r_{n,|\ell|}\rangle = \sqrt{2}\lambda\sum_{k=0}^{n}\sum_{j=0}^{n-k}\frac{(-2)^j(n + |\ell| + k)!\Gamma(|\ell| + 2k + j + \frac{3}{2})}{k!j!(|\ell| + k)!(n - k - j)!(|\ell| + 2k + j)!}, \tag{78}$$

$$\langle p_\perp^2\rangle = \tfrac{1}{2}eB\hbar(2n + 1 + |\ell|), \tag{79}$$

$$\langle r_1^2\rangle = \lambda^2(2n + 1), \tag{80}$$

$$\langle r_0^2\rangle = \lambda^2\{2(n + \ell) + 1\}, \tag{81}$$

where Γ is the gamma function.

V. MATRIX ELEMENTS

In this last section we proceed to the calculation of the matrix elements which will be needed in Paper II for the treatment of the conductivity tensor. We choose to work with eigenfunctions of the set of commuting operators H, p_x, and p_z in the gauge $\mathbf{A} = -By\hat{i}$, namely Eqs. (54) and (55). This is because the matrix elements in this system take the simplest form in comparison with the other possible choices. The matrix elements are written symbolically $\langle\epsilon',p'|O|\epsilon,p\rangle$, where p denotes the set of quantum numbers $\{p_x,p_z,\nu\}$ and ϵ a particle or an antiparticle state.

The conductivity tensor $\overleftrightarrow{\sigma}$ is defined as the linear response tensor relating the Fourier–Laplace transformed perturbations $\mathbf{j}_1$ in the current density induced by the perturbations $\mathbf{E}_1$ in the electric field:

$$\mathbf{j}_1(\mathbf{q},\omega) = \sum_{\mathbf{q}'}\overleftrightarrow{\sigma}(\mathbf{q},\mathbf{q}',\omega)\cdot\mathbf{E}_1(\mathbf{q}',\omega), \tag{82}$$

where $\mathbf{q}'$ and $\mathbf{q}$ are wavenumbers and ω is the angular frequency. In the case of a boson–antiboson plasma in a strong magnetic field the conductivity tensor has the following form[7]:

$$\begin{aligned}\overleftrightarrow{\sigma}(\mathbf{q},\mathbf{q}',\omega) &= \frac{ie^2}{m\hbar V}\sum_{\epsilon',p'}\sum_{\epsilon,p}\left[\frac{\epsilon F_{\epsilon'}(p')-\epsilon' F_{\epsilon}(p)}{\omega-(1/\hbar)[\epsilon E_\nu-\epsilon' E_{\nu'}]+i\eta}\right] \\ &\times\langle\epsilon',p'|\tau_0 e^{-i\mathbf{q}\cdot\mathbf{r}}(\pi-\tfrac{1}{2}\hbar\mathbf{q})|\epsilon,p\rangle \\ &\times\left\{\begin{matrix}\langle\epsilon,p|e^{i\mathbf{q}'\cdot\mathbf{r}}|\epsilon',p'\rangle(\mathbf{q}'/q'^2) \\ +(1/m\omega)\langle\epsilon,p|\tau_0 e^{i\mathbf{q}'\cdot\mathbf{r}}\pi|\epsilon',p'\rangle\cdot\overleftrightarrow{\mathbf{I}}'\end{matrix}\right\} \\ &+\frac{ie^2}{m\omega V}\sum_{\epsilon,p}F_\epsilon(p)\langle\epsilon,p|\tau_0 e^{i(\mathbf{q}'-\mathbf{q})\cdot\mathbf{r}}|\epsilon,p\rangle\overleftrightarrow{\mathbf{I}}'. \qquad (83)\end{aligned}$$

Here $\overleftrightarrow{\mathbf{I}}'$ is the projection tensor $\overleftrightarrow{\mathbf{I}}-\mathbf{q}'\mathbf{q}'/q'^2$, $F_+(p)$ is the boson equilibrium distribution function $N_+(p)$ and $F_-(p)=1+N_-(p)$ where $N_-(p)$ is the antiboson equilibrium distribution function. Here V is the volume of the system and η is an infinitesimal introduced in the Landau procedure ensuring that the perturbations vanish as $t\to-\infty$.

From this expression it is clear that three distinct types of matrix elements are required for the evaluation of the conductivity tensor:

(a) $\langle\epsilon',p'|e^{i\mathbf{q}\cdot\mathbf{r}}|\epsilon,p\rangle$,

(b) $\langle\epsilon',p'|\tau_0 e^{i\mathbf{q}\cdot\mathbf{r}}|\epsilon,p\rangle$,

(c) $\langle\epsilon',p'|\tau_0 e^{i\mathbf{q}\cdot\mathbf{r}}\pi|\epsilon,p\rangle$.

A. Evaluation of $\langle\epsilon',p'|e^{i\mathbf{q}\cdot\mathbf{r}}|\epsilon,p\rangle$

In this case the x and z integrations are trivial, yielding Kronecker deltas, and there remains a y integral:

$$\begin{aligned}&\langle\epsilon',p'|e^{i\mathbf{q}\cdot\mathbf{r}}|\epsilon,p\rangle \\ &=\frac{\epsilon E_\nu+\epsilon' E_{\nu'}}{2\sqrt{E_\nu E_{\nu'}}}\delta_{\epsilon' p'_x,\epsilon p_x+\hbar q_x}\delta_{\epsilon' p'_z,\epsilon p_z+\hbar q_z} \\ &\times[\pi 2^{\nu+\nu'}\nu!\nu'!]^{-1/2} \\ &\times\int_{-\infty}^{\infty}\exp\left[i\gamma u-\frac{1}{2}(u-u'_0)^2-\frac{1}{2}(u-u_0)^2\right] \\ &\times H_{\nu'}(u-u'_0)H_\nu(u-u_0)du, \qquad (84)\end{aligned}$$

where $\gamma\equiv\lambda q_y$, $u_0\equiv\epsilon y_0/\lambda$, $u'_0\equiv\epsilon' y'_0/\lambda$, and $u\equiv y/\lambda$. This integral has appeared in studies of the dielectric response of an electron plasma in a strong magnetic field and has been evaluated in Appendix B of Delsante and Frankel.[12] It is

$$\begin{aligned}&\pi^{1/2}2^{\nu'}\nu'!(-1)^{\nu-\nu'}[\lambda q_\perp]^{\nu-\nu'} \\ &\times\exp\left\{-\frac{\lambda^2 q_\perp^2}{4}+i(\nu'-\nu)\phi-\frac{iq_y(2\epsilon p_x+\hbar q_x)}{2eB}\right\} \\ &\times L_{\nu'}^{\nu-\nu'}\left(\frac{\lambda^2 q_\perp^2}{2}\right)\quad\text{if }\nu\geq\nu' \qquad (85a)\end{aligned}$$

and

$$\begin{aligned}&\pi^{1/2}2^{\nu}\nu![\lambda q_\perp]^{\nu'-\nu} \\ &\times\exp\left\{-\frac{\lambda^2 q_\perp^2}{4}+i(\nu'-\nu)\phi-\frac{iq_y(2\epsilon p_x+\hbar q_x)}{2eB}\right\} \\ &\times L_{\nu}^{\nu'-\nu}\left(\frac{\lambda^2 q_\perp^2}{2}\right)\quad\text{if }\nu'\geq\nu. \qquad (85b)\end{aligned}$$

In these expressions $q_x=q_\perp\cos\phi$, $q_y=q_\perp\sin\phi$, and $L_\nu^{\nu'-\nu}$, $L_{\nu'}^{\nu-\nu'}$ are generalized Laguerre polynomials.

The integral appearing in Eq. (84) [the standard evaluation resulting in Eqs. (85a) and (85b)] may be obtained more directly by the following procedure. We define

$$\begin{aligned}q_+&\equiv q_x+iq_y=q_\perp e^{i\phi},\\ q_-&\equiv q_x-iq_y=q_\perp e^{-i\phi},\\ q_\perp^2&=q_x^2+q_y^2\end{aligned}$$

and substitute into the integral of Eq. (84) which becomes

$$\begin{aligned}&\exp\left\{-\frac{i\epsilon p_x q_y}{eB}\right\}\int_{-\infty}^{\infty}du \\ &\times\exp\{i\lambda q_y u-u^2-u\lambda q_x-\tfrac{1}{2}\lambda^2 q_x^2\} \\ &\times H_{\nu'}(u)H_\nu(u+q_x),\end{aligned}$$

where the origin has been shifted by use of the transformation

$$u\to u+\epsilon p_x/eB\lambda.$$

From the generating function one may define the integral representation

$$H_n(x)=\frac{n!}{2\pi i}\oint_c\frac{dz}{z^{n+1}}e^{2xz-z^2},$$

where c is any contour encircling the origin. The integral then becomes

$$\begin{aligned}&\frac{\nu!\nu'!}{(2\pi i)^2}\exp\left\{-\frac{i\epsilon p_x q_y}{eB}-\frac{1}{2}\lambda^2 q_x^2\right\} \\ &\times\oint\frac{dz}{z^{\nu+1}}\oint\frac{dz'}{z'^{\nu'+1}} \\ &\times\exp\{-z^2-z'^2+2\lambda q_x z'\} \\ &\times\int_{-\infty}^{\infty}du\exp\{-u^2+u(i\lambda q_y-\lambda q_x+2(z+z'))\}\end{aligned}$$

and the entire integral may be written, after doing the u integration, in the form

$$\begin{aligned}&\frac{\pi^{1/2}\nu!\nu'!}{(2\pi i)^2}\exp\left\{-\frac{1}{4}\lambda^2 q_\perp^2-\frac{iq_y}{2eB}(2\epsilon p_x+\hbar q_x)\right\} \\ &\times\oint\frac{dz}{z^{\nu+1}}\exp\{-\lambda z q_-\} \\ &\times\oint\frac{dz'}{z'^{\nu'+1}}\exp\{z'(2z+\lambda q_+)\}.\end{aligned}$$

In the z' integral, let $s'\equiv z'[2z+\lambda q_+]$. Then

$$\begin{aligned}&\frac{1}{2\pi i}\oint_c\frac{dz'}{z'^{\nu'+1}}\exp\{z'(\lambda q_+ +2z)\} \\ &\quad=[2z+\lambda q_+]^{\nu}\frac{1}{2\pi i}\oint_c\frac{ds'}{s'^{\nu'+1}}e^{s'}\end{aligned}$$

and the contour c is deformed so that the integral becomes

$$\frac{1}{2\pi i}\int_{-\infty}^{(0^+)}\frac{ds'\,e^{s'}}{s'^{\nu'+1}}=\frac{1}{\Gamma(\nu'+1)}=\frac{1}{\nu'!}$$

(Hankel's integral formula). We are left with

$$\pi^{1/2}\nu!\exp\left\{-\frac{1}{4}\lambda^2 q_\perp^2-\frac{iq_y}{2eB}(2\epsilon p_x+\hbar q_x)\right\}$$

$$\times\frac{1}{2\pi i}\oint_c\frac{dz}{z^{\nu+1}}e^{-z\lambda q_-}[2z+\lambda q_+]^{\nu'}.$$

Focusing now on the last integral, we write $z=-\frac{1}{2}\lambda s q_+$ and transform the integral thus

$$\begin{aligned}&\frac{1}{2\pi i}\oint\frac{dz}{z^{\nu+1}}e^{-\lambda z q_-}[2z+\lambda q_+]^{\nu'}\\&=\left(-\frac{1}{2}\lambda q_+\right)^{\nu'-\nu}\left(\frac{1}{2\pi i}\right)\\&\times\oint_c\frac{ds}{s^{\nu+1}}e^{(1/2)\lambda^2 q_\perp^2 s}[2s-2]^{\nu'}\\&=2^{\nu}(-1)^{\nu'-\nu}(\lambda q_+)^{\nu'-\nu}\left(\frac{1}{2\pi i}\right)\\&\times\oint\frac{ds}{s^{\nu+1}}e^{(1/2)\lambda^2 q_\perp^2 s}[s-1]^{\nu'}.\end{aligned}$$

One can show from the differential equation of the Laguerre polynomials that

$$L_\nu^{\nu'-\nu}(x)=\frac{(-1)^{\nu'-\nu}}{2\pi i}\int_{c-i\infty}^{c+i\infty}\frac{ds}{s^{\nu+1}}e^{sx}(s-1)^{\nu'},$$

where $x>0$, $c>0$, and $\nu'\geqslant\nu$.

Now, deform the contour parallel to the imaginary axis into a circle enclosing the origin, finally arriving at

$$\begin{aligned}&\frac{1}{2\pi i}\oint\frac{dz}{z^{\nu+1}}e^{-\lambda z q_-}[2z+\lambda q_+]^{\nu'}\\&\quad=2^{\nu}(\lambda q_+)^{\nu'-\nu}L_\nu^{\nu'-\nu}(\tfrac{1}{2}\lambda^2 q_\perp^2).\end{aligned}$$

The integral then becomes precisely the result (85b). To derive the other case, $\nu\geqslant\nu'$, one integrates the z integral first, this time with $s=z(-\lambda q_-+2z')$, to obtain

$$\begin{aligned}&\frac{1}{2\pi i}\oint\frac{dz}{z^{\nu+1}}\exp\{-\lambda z q_-+2zz'\}\\&\quad=\frac{(-\lambda q_-+2z')^{\nu}}{2\pi i}\int_{-\infty}^{(O^+)}\frac{ds\,e^s}{s^{\nu+1}}\\&\quad=\frac{(2z'-\lambda q_-)^{\nu}}{\nu!}.\end{aligned}$$

The remaining z' integral, using the substitution $z'=\frac{1}{2}\lambda q_- s'$, becomes

$$\begin{aligned}&\frac{1}{2\pi i}\oint\frac{dz'}{z'^{\nu'+1}}e^{\lambda q_+ z'}[2z'-\lambda q_-]^{\nu}\\&\quad=\frac{1}{2\pi i}\left(\frac{1}{2}\lambda q_-\right)^{\nu-\nu'}\int_{c-i\infty}^{c+i\infty}\frac{ds'\,e^{(1/2)\lambda^2 q_\perp^2 s'}}{s'^{\nu'+1}}[2s'-2]^{\nu}\\&\quad=2^{\nu'}(\lambda q_-)^{\nu-\nu'}(-1)^{\nu-\nu'}L_{\nu'}^{\nu-\nu'}(\tfrac{1}{2}\lambda^2 q_\perp^2),\end{aligned}$$

which results immediately in Eq. (85a).

Since all matrix elements will be linear combinations of integrals of the type just discussed, the following functions are defined:

$$\beta_{\nu'\nu}(\boldsymbol{\mu})=e^{-(1/4)\mu_\perp^2}e^{i(\nu'-\nu)\phi}\alpha_{\nu'\nu}(\mu_\perp)\tag{86}$$

and

$$\begin{aligned}&\alpha_{\nu'\nu}(\mu_\perp)\\&\quad=[2^{\nu}\nu!/2^{\nu'}\nu'!]^{1/2}\mu_\perp^{\nu'-\nu}L_\nu^{\nu'-\nu}(\tfrac{1}{2}\mu_\perp^2)\quad\text{if }\nu'\geqslant\nu\qquad(87a)\\&\quad=[2^{\nu'}\nu'!/2^{\nu}\nu!]^{1/2}(-1)^{\nu-\nu'}\mu_\perp^{\nu-\nu'}L_{\nu'}^{\nu-\nu'}(\tfrac{1}{2}\mu_\perp^2)\\&\quad\text{if }\nu\geqslant\nu',\qquad(87b)\end{aligned}$$

where $\boldsymbol{\mu}$ is a nondimensional wave vector $\lambda\mathbf{q}$. Useful properties of α and β that will be drawn upon are

$$\beta_{\nu'\nu}(-\boldsymbol{\mu})=(-1)^{\nu'-\nu}\beta_{\nu'\nu}(\boldsymbol{\mu})$$

and

$$\alpha_{\nu'\nu}(\mu_\perp)=(-1)^{\nu'-\nu}\alpha_{\nu\nu'}(\mu_\perp).$$

Note that $\beta_{\nu'\nu}\neq\beta_{\nu\nu'}$.

One important case is $\beta_{\nu'\nu}(0)=\alpha_{\nu'\nu}(0)=\delta_{\nu'\nu}$. In terms of this notation the scalar matrix element of this subsection becomes

$$\begin{aligned}\langle\epsilon',p'|e^{i\mathbf{q}\cdot\mathbf{r}}|\epsilon,p\rangle=&\frac{\epsilon' E_{\nu'}+\epsilon E_\nu}{2\sqrt{E_\nu E_{\nu'}}}\delta_{\epsilon' p_x',\epsilon p_x+\hbar q_x}\delta_{\epsilon' p_z',\epsilon p_z+\hbar q_z}\\&\times\exp\left\{-\frac{iq_y}{2eB}(2\epsilon p_x+\hbar q_x)\right\}\beta_{\nu'\nu}(\boldsymbol{\mu}).\end{aligned}\tag{88}$$

B. Evaluation of $\langle\epsilon',\mathbf{p}'|\tau_0 e^{i\mathbf{q}\cdot\mathbf{r}}|\epsilon,\mathbf{p}\rangle$

This matrix element differs from the first only by an energy factor and is

$$\begin{aligned}\langle\epsilon',p'|\tau_0 e^{i\mathbf{q}\cdot\mathbf{r}}|\epsilon,p\rangle=&\frac{mc^2}{\sqrt{E_\nu E_{\nu'}}}\delta_{\epsilon' p_x',\epsilon p_x+\hbar q_x}\delta_{\epsilon' p_z',\epsilon p_z+\hbar q_z}\\&\times\exp\left\{-\frac{iq_y}{2eB}(2\epsilon p_x+\hbar q_x)\right\}\beta_{\nu'\nu}(\boldsymbol{\mu}).\end{aligned}\tag{89}$$

C. Evaluation of $\langle\epsilon',\mathbf{p}'|\tau_0 e^{i\mathbf{q}\cdot\mathbf{r}}\boldsymbol{\pi}|\epsilon,\mathbf{p}\rangle$

The π_z component of this vector matrix element is particularly simple,

$$\langle\epsilon',p'|\tau_0 e^{i\mathbf{q}\cdot\mathbf{r}}\pi_z|\epsilon,p\rangle=\epsilon p_z\langle\epsilon',p'|\tau_0 e^{i\mathbf{q}\cdot\mathbf{r}}|\epsilon,p\rangle,\tag{90}$$

while the two other components take different forms. These can be calculated in a number of ways. The most transparent method uses the ladder operators π_+,π_- in Eqs. (47a) and (47b):

$$\begin{aligned}&\langle\epsilon',p',\nu'|\tau_0 e^{i\mathbf{q}\cdot\mathbf{r}}\pi_x|\epsilon,p,\nu\rangle\\&\quad=\frac{\hbar}{\lambda}\left(\frac{(\nu+1)E_{\nu+1}}{2E_\nu}\right)^{1/2}\langle\epsilon',p',\nu'|\tau_0 e^{i\mathbf{q}\cdot\mathbf{r}}|\epsilon,p,\nu+1\rangle\\&\quad+\frac{\hbar}{\lambda}\left(\frac{\nu E_{\nu-1}}{2E_\nu}\right)^{1/2}\langle\epsilon',p',\nu'|\tau_0 e^{i\mathbf{q}\cdot\mathbf{r}}|\epsilon,p,\nu-1\rangle\end{aligned}\tag{91a}$$

and

$$\begin{aligned}&\langle\epsilon',p',\nu'|\tau_0 e^{i\mathbf{q}\cdot\mathbf{r}}\pi_y|\epsilon,p,\nu\rangle\\&\quad=\frac{\hbar}{i\lambda}\left(\frac{\nu E_{\nu-1}}{2E_\nu}\right)^{1/2}\langle\epsilon',p',\nu'|\tau_0 e^{i\mathbf{q}\cdot\mathbf{r}}|\epsilon,p,\nu-1\rangle\\&\quad-\frac{\hbar}{i\lambda}\left(\frac{(\nu+1)E_{\nu+1}}{2E_\nu}\right)^{1/2}\langle\epsilon',p',\nu'|\tau_0 e^{i\mathbf{q}\cdot\mathbf{r}}|\epsilon,p,\nu+1\rangle.\end{aligned}\tag{91b}$$

Alternatively, one can use the completeness relation to form an expansion in terms of the matrix elements of the individual operators for any two unit matrix operators A and B,

$$\langle\alpha|\tau_0 AB|\beta\rangle = \sum_\gamma \frac{2\epsilon_\gamma E_\gamma}{\epsilon_\gamma E_\gamma + \epsilon_\beta E_\beta}\langle\alpha|\tau_0 A|\gamma\rangle\langle\gamma|B|\beta\rangle. \quad (92)$$

This follows from Eq. (58) and thus

$$\langle\epsilon',p'|\tau_0 e^{iq\cdot r}\pi_x|\epsilon,p\rangle = \sum_{\epsilon'',p''}\frac{2\epsilon'' E''}{\epsilon'' E'' + \epsilon E}\langle\epsilon',p'|\tau_0 e^{iq\cdot r}|\epsilon'',p''\rangle \times\langle\epsilon'',p''|(p_x + eBy)|\epsilon,p\rangle \quad (93)$$

and

$$\langle\epsilon',p'|\tau_0 e^{iq\cdot r}\pi_y|\epsilon,p\rangle = \sum_{\epsilon'',p''}\frac{2\epsilon'' E''}{\epsilon'' E'' + \epsilon E}\langle\epsilon',p'|\tau_0 e^{iq\cdot r}|\epsilon'',p''\rangle \times\langle\epsilon'',p''|p_y|\epsilon,p\rangle. \quad (94)$$

The two subsidiary matrix elements are

$$\langle\epsilon',p'|y|\epsilon,p\rangle = \frac{\epsilon' E_{\nu'} + \epsilon E_\nu}{2\sqrt{E_\nu E_{\nu'}}}\delta_{\epsilon,\epsilon'}\delta_{p,p'} \times\left[\epsilon y_0\delta_{\nu',\nu} + \lambda\sqrt{\nu+1}\,\delta_{\nu',\nu+1} + \lambda\sqrt{\nu}\,\delta_{\nu',\nu-1}\right] \quad (95)$$

and

$$\langle\epsilon',p'|p_y|\epsilon,p\rangle = \frac{\epsilon' E_{\nu'} + \epsilon E_\nu}{2\sqrt{E_\nu E_{\nu'}}}\delta_{\epsilon',\epsilon}\delta_{p',p} \times\frac{\hbar}{\lambda}\left[i\sqrt{\frac{\nu+1}{2}}\,\delta_{\nu',\nu+1} - i\sqrt{\frac{\nu}{2}}\,\delta_{\nu',\nu-1}\right], \quad (96)$$

which, when inserted into the expansions [Eqs. (93) and (94)], give identical results with those found previously, namely,

$$\langle\epsilon',p',\nu'|\tau_0 e^{iq\cdot r}\pi_x|\epsilon,p,\nu\rangle = \frac{\hbar mc^2}{\lambda\sqrt{E_\nu E_{\nu'}}}\delta_{\epsilon' p'_x,\epsilon p_x+\hbar q_x}\delta_{\epsilon' p'_z,\epsilon p_z+\hbar q_z} \times\exp\left[-\frac{iq_y}{2eB}(2\epsilon p_x + \hbar q_x)\right] \times\left(\sqrt{\frac{\nu+1}{2}}\,\beta_{\nu',\nu+1} + \sqrt{\frac{\nu}{2}}\,\beta_{\nu',\nu-1}\right) \quad (97)$$

and

$$\langle\epsilon',p',\nu'|\tau_0 e^{iq\cdot r}\pi_y|\epsilon,p,\nu\rangle = \frac{\hbar mc^2}{\lambda\sqrt{E_\nu E_{\nu'}}}\delta_{\epsilon' p'_x,\epsilon p_x+\hbar q_x}\delta_{\epsilon' p'_z,\epsilon p_z+\hbar q_z} \times\exp\left[-\frac{iq_y}{2eB}(2\epsilon p_x + \hbar q_x)\right] \times\left(i\sqrt{\frac{\nu+1}{2}}\,\beta_{\nu',\nu+1} - i\sqrt{\frac{\nu}{2}}\,\beta_{\nu',\nu-1}\right). \quad (98)$$

So far the matrix elements of π_x and π_y have been taken between states where the transverse quantum number ν is raised or lowered one unit. We will also find it necessary to write these matrix elements in a form where the other subscript ν' is raised or lowered. This other form is found by considering the generalized Hermitian conjugate operator

$$\langle\epsilon',p'|\tau_0 e^{iq\cdot r}\pi|\epsilon,p\rangle = \langle\epsilon,p|(\tau_0 e^{iq\cdot r}\pi)^\ddagger|\epsilon',p'\rangle^* = \langle\epsilon,p|\tau_0\pi e^{-iq\cdot r}|\epsilon',p'\rangle^* \quad (99)$$

and recognizing that π is Hermitian and $\tau_3\tau_0^\dagger\tau_3 = \tau_0$. Taking each component in turn we find

$$\langle\epsilon',p',\nu'|\tau_0 e^{iq\cdot r}\pi_z|\epsilon,p,\nu\rangle = (\epsilon' p'_z - \hbar q_z)\langle\epsilon',p',\nu'|\tau_0 e^{iq\cdot r}|\epsilon,p,\nu\rangle, \quad (100)$$

$$\langle\epsilon',p',\nu'|\tau_0 e^{iq\cdot r}\pi_x|\epsilon,p,\nu\rangle = -\hbar q_x\langle\epsilon',p',\nu'|\tau_0 e^{iq\cdot r}|\epsilon,p,\nu\rangle + \frac{\hbar}{\lambda}\left(\frac{(\nu'+1)E_{\nu'+1}}{2E_{\nu'}}\right)^{1/2}\langle\epsilon',p',\nu'+1|\tau_0 e^{iq\cdot r}|\epsilon,p,\nu\rangle + \frac{\hbar}{\lambda}\left(\frac{\nu' E_{\nu'-1}}{2E_{\nu'}}\right)^{1/2}\langle\epsilon',p',\nu'-1|\tau_0 e^{iq\cdot r}|\epsilon,p,\nu\rangle, \quad (101)$$

and

$$\langle\epsilon',p',\nu'|\tau_0 e^{iq\cdot r}\pi_y|\epsilon,p,\nu\rangle = -\hbar q_y\langle\epsilon',p',\nu'|\tau_0 e^{iq\cdot r}|\epsilon,p,\nu\rangle - \frac{i\hbar}{\lambda}\left(\frac{(\nu'+1)E_{\nu'+1}}{2E_{\nu'}}\right)^{1/2}\langle\epsilon',p',\nu'+1|\tau_0 e^{iq\cdot r}|\epsilon,p,\nu\rangle + \frac{i\hbar}{\lambda}\left(\frac{\nu' E_{\nu'-1}}{2E_{\nu'}}\right)^{1/2}\langle\epsilon',p',\nu'-1|\tau_0 e^{iq\cdot r}|\epsilon,p,\nu\rangle. \quad (102)$$

Again the same result can be achieved by using the completeness relation in the form

$$\langle\epsilon',p'|\tau_0\pi e^{iq\cdot r}|\epsilon,p\rangle = \sum_{\epsilon'',p''}\frac{2\epsilon'' E''}{\epsilon'' E'' + \epsilon E}\langle\epsilon',p'|\pi|\epsilon'',p''\rangle \times\langle\epsilon'',p''|\tau_0 e^{iq\cdot r}|\epsilon,p\rangle. \quad (103)$$

The form in which these matrix elements will be used is

$$\langle\epsilon',p',\nu'|\tau_0 e^{iq\cdot r}\pi_x|\epsilon,p,\nu\rangle = \frac{mc^2}{\sqrt{E_\nu E_{\nu'}}}\delta_{\epsilon' p'_x,\epsilon p_x+\hbar q_x}\delta_{\epsilon' p'_z,\epsilon p_z+\hbar q_z} \times\exp\left[-\frac{iq_y}{2eB}(2\epsilon p_x + \hbar q_x)\right] \times\frac{\hbar}{\lambda}\left[-\mu_x\beta_{\nu'\nu}(\mu) + \sqrt{\frac{\nu'+1}{2}}\,\beta_{\nu'+1,\nu}(\mu) + \sqrt{\frac{\nu'}{2}}\,\beta_{\nu'-1,\nu}(\mu)\right], \quad (104)$$

$$\langle\epsilon',p',\nu'|\tau_0 e^{iq\cdot r}\pi_y|\epsilon,p,\nu\rangle = \frac{mc^2}{\sqrt{E_\nu E_{\nu'}}}\delta_{\epsilon' p'_x,\epsilon p_x+\hbar q_x}\delta_{\epsilon' p'_z,\epsilon p_z+\hbar q_z} \times\exp\left[-\frac{iq_y}{2eB}(2\epsilon p_x + \hbar q_x)\right]$$

$$\times\frac{\hbar}{\lambda}\left[-\mu_y\beta_{\nu',\nu}(\mu)-i\sqrt{\frac{\nu'+1}{2}}\beta_{\nu'+1,\nu}(\mu)\right.$$

$$\left.+i\sqrt{\frac{\nu}{2}}\beta_{\nu'-1,\nu}(\mu)\right]. \tag{105}$$

Obviously these two alternative means of expressing the matrix elements will establish a relationship between $\alpha_{\nu',\nu}$ and $\alpha_{\nu'\pm1,\nu}$ on the one hand and $\alpha_{\nu',\nu\pm1}$ on the other hand. These relationships, derived in the Appendix, are

$$\frac{1}{2}\mu_\perp\alpha_{\nu',\nu}=\sqrt{\frac{\nu'+1}{2}}\alpha_{\nu'+1,\nu}-\sqrt{\frac{\nu}{2}}\alpha_{\nu',\nu-1}, \tag{106a}$$

$$\frac{1}{2}\mu_\perp\alpha_{\nu',\nu}=-\sqrt{\frac{\nu+1}{2}}\alpha_{\nu',\nu+1}+\sqrt{\frac{\nu'}{2}}\alpha_{\nu'-1,\nu}, \tag{106b}$$

and result from the definition of the $\alpha_{\nu',\nu}$ in terms of Laguerre polynomials.

In summary, the matrix elements that are specifically required in Paper II for the conductivity tensor are

$$\langle\epsilon',p',\nu'|\tau_0 e^{-i\mathbf{q}\cdot\mathbf{r}}\begin{Bmatrix}\pi_x\\ \pi_y\\ \pi_z\end{Bmatrix}|\epsilon,p,\nu\rangle=\frac{mc^2}{\sqrt{E_\nu E_{\nu'}}}\delta_{\epsilon'p'_x,\epsilon p_x-\hbar q_x}\delta_{\epsilon'p'_z,\epsilon p_z-\hbar q_z}\exp\left\{\frac{iq_y}{2eB}(2\epsilon p_x-\hbar q_x)\right\}$$

$$\times\begin{Bmatrix}\frac{\hbar}{\lambda}\left[\sqrt{\frac{\nu+1}{2}}\beta_{\nu',\nu+1}(-\mu)+\sqrt{\frac{\nu}{2}}\beta_{\nu',\nu-1}(-\mu)\right]\\ \frac{\hbar}{\lambda}\left[i\sqrt{\frac{\nu+1}{2}}\beta_{\nu',\nu+1}(-\mu)-i\sqrt{\frac{\nu}{2}}\beta_{\nu',\nu-1}(-\mu)\right]\\ \epsilon p_z\beta_{\nu',\nu}(-\mu)\end{Bmatrix}, \tag{107}$$

$$\langle\epsilon,p,\nu|\tau_0 e^{i\mathbf{q}'\cdot\mathbf{r}}\begin{Bmatrix}\pi_x\\ \pi_y\\ \pi_z\end{Bmatrix}|\epsilon',p',\nu'\rangle=\frac{mc^2}{\sqrt{E_\nu E_{\nu'}}}\delta_{\epsilon p_x,\epsilon'p'_x+\hbar q'_x}\delta_{\epsilon p_z,\epsilon'p'_z+\hbar q'_z}\exp\left\{-\frac{iq'_y}{2eB}(2\epsilon'p'_x+\hbar q'_x)\right\}$$

$$\times\begin{Bmatrix}\frac{\hbar}{\lambda}\left[-\mu'_x\beta_{\nu,\nu'}(\mu')+\sqrt{\frac{\nu+1}{2}}\beta_{\nu+1,\nu'}(\mu')+\sqrt{\frac{\nu}{2}}\beta_{\nu-1,\nu'}(\mu')\right]\\ \frac{\hbar}{\lambda}\left[-\mu'_y\beta_{\nu,\nu'}(\mu')-i\sqrt{\frac{\nu+1}{2}}\beta_{\nu+1,\nu'}(\mu')+i\sqrt{\frac{\nu}{2}}\beta_{\nu-1,\nu'}(\mu')\right]\\ (\epsilon p_z-\hbar q'_z)\beta_{\nu,\nu'}(\mu')\end{Bmatrix}, \tag{108}$$

$$\langle\epsilon,p,\nu|e^{i\mathbf{q}'\cdot\mathbf{r}}|\epsilon',p',\nu'\rangle$$
$$=\frac{\epsilon E_\nu+\epsilon' E_{\nu'}}{2\sqrt{E_\nu E_{\nu'}}}\delta_{\epsilon p_x,\epsilon'p'_x+\hbar q'_x}\delta_{\epsilon p_z,\epsilon'p'_z+\hbar q'_z}$$
$$\times\exp\left\{-\frac{iq'_y}{2eB}(2\epsilon'p'_x+\hbar q'_x)\right\}\beta_{\nu,\nu'}(\mu') \tag{109}$$

and

$$\langle\epsilon,p|\tau_0 e^{i(\mathbf{q}'-\mathbf{q})\cdot\mathbf{r}}|\epsilon',p'\rangle$$
$$=\frac{mc^2}{E_\nu}\delta_{q'_x,q_x}\delta_{q'_z,q_z}$$
$$\times\exp\left\{-\frac{i(q'_y-q_y)\epsilon p_x}{eB}\right\}\beta_{\nu,\nu'}(\mu'-\mu). \tag{110}$$

VI. CONCLUSION

With the calculation of these matrix elements we conclude this preliminary paper in our series of three. We have so far given a thorough treatment of the Klein–Gordon equation in the presence of a strong magnetic field and employed the resulting wave functions to calculate the various matrix elements detailed in the previous section.

Although in Paper II [7] these matrix elements will be needed in the derivation and reduction of the conductivity tensor appropriate to a boson–antiboson plasma in an intense magnetic field, it is worth noting here that their utility is by no means restricted to this particular application. The matrix elements evaluated in Sec. V would also appear in any kinetic equation introduced to handle transport processes in the boson–antiboson plasma and in investigations of the screening properties of such a system. It is also worth mentioning that almost identical matrix elements are encountered when radiation transport in a system of this nature is considered, that is to say, for all problems involving the emission and absorption of photons. As discussed by Canuto and Ventura[13] these sorts of matrix elements occur whenever collisional processes between component particles of the plasma are important. Although Canuto and Ventura confine their considerations to the nonrelativistic fermion plasma, the extensions to which they refer are equally valid for the systems under discussion in the present work.

So far as the succeeding papers are concerned, Paper II is devoted to a comprehensive investigation of the conductivity and dielectric tensors for a boson–antiboson plasma. After the derivation of the form of the conductivity tensor,

we discuss the zero field limit of the tensor elements. For the general case of nonzero field, the tensor is reduced and simplified to a particularly tractable form. We consider also the long wavelength limit and, most important for comparison with the earlier work, the zero temperature limit. The detailed comparison with the fermion work highlights the important differences between the two systems.

Paper III in the series is entirely concerned with a detailed study of the vacuum properties of the conductivity and dielectric tensors. The complete renormalization program is carried through for the first time in the boson case and two representations are presented of the renormalized tensor. These unify different approaches which have been used in the past for the fermion case. The static and dynamic polarizabilities of the magnetized boson vacuum are investigated both analytically and numerically and compared with the equivalent fermion results.

APPENDIX: α FUNCTION IDENTITIES

(a) The fundamental relationships between $\alpha_{\nu'\pm1,\nu}$, $\alpha_{\nu',\nu}$, and $\alpha_{\nu',\nu\pm1}$ in Eq. (106) can be established by equating the alternative expressions for the matrix elements of π_x (or π_y). Here, however, we proceed to verify them directly from their definitions.

Considering, first, Eq. (106a) there are two distinct cases.

(i) $\nu'+1\geqslant\nu$:

$$\sqrt{\frac{\nu'+1}{2}}\,\alpha_{\nu'+1,\nu}-\sqrt{\frac{\nu}{2}}\,\alpha_{\nu',\nu-1}=\frac{1}{2}\left[\frac{2^\nu\nu!}{2^{\nu'}\nu'!}\right]^{1/2}\mu_\perp^{\nu'-\nu+1}\left[L_\nu^{\nu'+1-\nu}-L_{\nu-1}^{\nu'-\nu+1}\right]. \tag{A1}$$

Now $L_\nu^{\nu'-\nu+1}-L_{\nu-1}^{\nu'-\nu+1}=L_\nu^{\nu'-\nu}$ so that the required relation is

$$\sqrt{\frac{\nu'+1}{2}}\,\alpha_{\nu'+1,\nu}-\sqrt{\frac{\nu}{2}}\,\alpha_{\nu',\nu-1}=\frac{1}{2}\mu_\perp\alpha_{\nu'\nu}. \tag{A2}$$

(ii) $\nu\geqslant\nu'+1$:

$$\sqrt{\frac{\nu'+1}{2}}\,\alpha_{\nu'+1,\nu}-\sqrt{\frac{\nu}{2}}\,\alpha_{\nu',\nu-1}=\left[\frac{2^{\nu'}\nu'!}{2^\nu\nu!}\right]^{1/2}(-1)^{\nu'-\nu+1}\mu^{\nu-\nu'+1}\times\left[(\nu'+1)L_{\nu'+1}^{\nu-\nu'-1}-\nu L_\nu^{\nu-1-\nu'}\right]. \tag{A3}$$

This time

$$(\nu'+1)L_{\nu'+1}^{\nu-\nu'-1}(\tfrac{1}{2}\mu_\perp^2)-\nu L_\nu^{\nu-1-\nu'}(\tfrac{1}{2}\mu_\perp^2)=-\tfrac{1}{2}\mu_\perp^2L_\nu^{\nu-\nu'}(\tfrac{1}{2}\mu_\perp^2) \tag{A4}$$

and we arrive at the same result as above.

The other identity, Eq. (106b), can be treated in the same way.

(iii) $\nu'-1\geqslant\nu$:

$$\sqrt{\frac{\nu+1}{2}}\,\alpha_{\nu',\nu+1}-\sqrt{\frac{\nu'}{2}}\,\alpha_{\nu'-1,\nu}=\left[\frac{2^\nu\nu!}{2^{\nu'}\nu'!}\right]^{1/2}\mu_\perp^{\nu'-\nu-1}\times\left[(\nu+1)L_{\nu+1}^{\nu'-\nu-1}-\nu'L_\nu^{\nu'-\nu-1}\right]=-\tfrac{1}{2}\mu_\perp\alpha_{\nu',\nu}. \tag{A5a}$$

(iv) $\nu\geqslant\nu'-1$:

$$\sqrt{\frac{\nu+1}{2}}\,\alpha_{\nu',\nu+1}-\sqrt{\frac{\nu'}{2}}\,\alpha_{\nu'-1,\nu}=\frac{1}{2}\left[\frac{2^{\nu'}\nu'!}{2^\nu\nu!}\right]^{1/2}(-1)^{\nu'-\nu-1}\mu_\perp^{\nu-\nu'+1}\times\left[L_\nu^{\nu-\nu'+1}-L_{\nu'-1}^{\nu-\nu'+1}\right]=-\tfrac{1}{2}\mu_\perp\alpha_{\nu',\nu}. \tag{A5b}$$

These two identities [Eqs. (106a) and (106b)] can be combined in a particularly useful way by rewriting them as

$$\frac{1}{2}\mu_\perp\alpha_{\nu',\nu-1}=-\sqrt{\frac{\nu}{2}}\,\alpha_{\nu',\nu}+\sqrt{\frac{\nu'}{2}}\,\alpha_{\nu'-1,\nu-1} \tag{A6a}$$

and

$$\frac{1}{2}\mu_\perp\alpha_{\nu'-1,\nu}=\sqrt{\frac{\nu'}{2}}\,\alpha_{\nu',\nu}-\sqrt{\frac{\nu}{2}}\,\alpha_{\nu'-1,\nu-1}. \tag{A6b}$$

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Field-diffeomorphism anomalies in the nonlinear σ model

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The field-diffeomorphism anomalies in the nonlinear σ model are explicitly discussed, using the spectral sequences technique. The role of the Riemannian constraints is analyzed for low space-time dimensions.

I. INTRODUCTION

We have nowadays become accustomed to applying the methods of algebraic topology to many current problems in quantum field theory (QFT). Thus magnetic monopoles, strings, instantons, solitons, anomalies, and so on, are typical subjects where the interaction between physicists and mathematicians has reached a remarkable level.[1]

In particular, the renormalization of models with symmetry has brought into evidence the power of cohomological methods,[2] which have provided a well-defined characterization of the role of the anomalies in QFT; indeed the anomalies obtained by lengthy Feynman diagram calculations were identified with the aid of precise theorems proved in the language of the algebraic topology. Anyhow, this powerful mathematical artillery sometimes has to be adapted for a more direct computational use, to the physicists requirements. Many authors[3–5] have emphasized the importance of this step, and recently we have fitted[6] the spectral sequences method[7–9] to the study of gauge and gravitational anomalies.

In this present paper we shall discuss and apply the same method to the renormalization of nonlinear σ models in which a local diffeomorphism invariance is present at the classical level. We shall see that this approach is practically insensitive to the nonpolynomiality of the model in the physical fields; however, to preserve the factorization of the manifold in which our model is defined into Faddeev–Popov ($\Phi\Pi$) charge eigenspaces, we shall require analyticity of the vertex operators in the $\Phi\Pi$ ghosts and their space-time derivatives.

In order to have a simple realization of the diffeomorphism algebra, we shall consider a parametrization of the models in terms of particular one-forms.

The cohomology problem then will be completely solved in the space of local functions, using the spectral sequences technique, and in the local functionals space for low space-time dimensions. We shall find anomalies in all the above cases, and we shall see that when the geometry of the manifold becomes Riemannian (which is not contained explicitly in the BRS operator), many anomalies vanish and only the ones analyzed in Refs. 10 and 11 survive.

In Sec. II we introduce the classical model and the notation.

Section III is devoted to the application of the spectral sequence technique to solve the cohomology problem in the space of the local functions.

In Sec. IV we discuss the cohomology of the BRS operator in the space of local functionals; we shall solve the problem for space-time dimension $d = 2,3,4$.

The Riemaniann geometry constraint is introduced in Sec. V, and its role in the trivialization of particular anomalies will be discussed.

Appendix A contains a summary of the spectral sequences technique, and we shall treat in detail the case where an infinite number of filtrations is needed to solve the problem.

Some technical aspects of Sec. II are discussed in Appendix B.

II. THE CLASSICAL MODEL

A nonlinear sigma model is a field theory in which the bosonic dynamical variables $\varphi^i(x)$ take their values in a manifold **M**. The dynamics of $\varphi^i(x)$ are determined by the classical action functional $\mathbf{S}(\varphi)$:

$$\mathbf{S}(\varphi) = \int_{\mathbf{R}} d^d x (\det g_{p\sigma}(x))^{1/2} g^{\mu\nu}(x) g_{ij}(\varphi(x)) \times \partial_\mu \varphi^j(x) \partial_\nu \varphi^j(x), \quad i,j = 1,...,n, \quad \mu,\nu = 1,...,d, \tag{2.1}$$

where **R** is the d-dimensional space-time endowed with the metric tensor $g^{\mu\nu}(x)$ and $g_{ij}(\varphi(x))$ is the metric on the target manifold **M**. The model is invariant under local fields diffeomormism $\mathcal{F}$ ($\mathcal{F}$ transformations),

$$\delta_{\mathcal{F}} \varphi^i(x) = \lambda^i(\varphi(x)), \tag{2.2}$$

such that

$$\delta_{\mathcal{F}} g_{ij}(\varphi(x)) = -\lambda_j{}^k(\varphi(x)) g_{ik}(\varphi(x)) - \lambda_i{}^k(\varphi(x)) g_{jk}(\varphi(x)), \tag{2.3}$$

where

$$\lambda^i{}_j(x) = \frac{\partial \lambda^i(\varphi(x))}{\partial \varphi^j(x)}. \tag{2.4}$$

Suppose that the metric tensors $g_{ij}(\varphi(x))$ and $g^{\mu\nu}(x)$ admit the vierbein decompositions

$$g_{ij}(\varphi(x)) = v_i{}^b(\varphi(x)) v_j{}^b(\varphi(x)), \tag{2.5}$$

$$g^{\mu\nu}(x) = e^\mu{}_a(x) e^\nu{}_a(x), \tag{2.6}$$

and introduce the quantity

$$V^b{}_a{}^i{}_j(\varphi(x)) = e^\mu{}_a(x) V^b{}_j(\varphi(x)) \partial_\mu \varphi^i(x) (\det g_{p\sigma}(x))^{1/4} \tag{2.7}$$

by means of which the action $\mathbf{S}(\varphi)$ is written

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$$S(\varphi)=\int_{\mathbf{R}} d^d x\, V^a{}_b{}^i{}_j(\varphi(x))V^b{}_a{}^j{}_i(\varphi(x)). \tag{2.8}$$

Under infinitesimal $\mathcal{F}$ transformations $V^a{}_b{}^i{}_j(\varphi(x))$ behaves as

$$\delta_{\mathcal{F}} V^b{}_a{}^i{}_j(\varphi(x))=\lambda^i{}_k(\varphi(x))V^b{}_a{}^k{}_j(\varphi(x)) - \lambda^k{}_j(\varphi(x))V^b{}_a{}^i{}_k(\varphi(x)). \tag{2.9}$$

In this paper we study the quantization of the model defined by means of the quantities $V^a{}_b{}^i{}_j(\varphi(x))$, as in Eq. (2.8).

Although this is not the most general parametrization, it greatly simplifies the procedure; and it can be useful for a first glance to the model and its geometrical setting.

In fact, if we consider the fields $\varphi^i(x)$ as coordinate of the model, the quantity $V^a{}_b{}^i{}_j(\varphi(x))$ can be interpreted as a one-form on the manifold M with values on the algebra of the $\mathcal{F}$ transformations.

The ordinary covariant derivative D_μ can be defined after the introduction of the local connection $\Gamma_\mu{}^i{}_j(\varphi(x))$,

$$D_\mu V^a{}_b{}^i{}_j(\varphi(x))=\partial_\mu V^a{}_b{}^i{}_j(\varphi(x))+\Gamma_\mu{}^k{}_j(\varphi(x))V^a{}_b{}^i{}_k(\varphi(x)) - \Gamma_\mu{}^i{}_k(\varphi(x))V^a{}_b{}^k{}_j(\varphi(x))$$

with

$$\delta_{\mathcal{F}}\Gamma_\mu{}^i{}_j((x))= -\lambda^i{}_k(\varphi(x))\Gamma_\mu{}^k{}_j(\varphi(x)) + \lambda^k{}_j((x))\Gamma_\mu{}^i{}_k(\varphi(x)) - \partial_\mu\lambda^i{}_j(\varphi(x)).$$

The algebra induced by the $\mathcal{F}$ transformations can be found by means of the operator D

$$D=\int d^d x\,\lambda^r{}_s(\varphi(x))D^s{}_r(x), \tag{2.10}$$

where we have denoted

$$D^s{}_r(x)=\left\{ -V^a{}_b{}^j{}_r(\varphi(x))\frac{\delta}{\delta V^a{}_b{}^j{}_s(\varphi(x))} + V^a{}_b{}^s{}_j(\varphi(x))\frac{\delta}{\delta V^a{}_b{}^r{}_j(\varphi(x))} - \Gamma_\mu{}^s{}_j(\varphi(x))\frac{\delta}{\delta\Gamma_\mu{}^r{}_j(\varphi(x))} + \Gamma_\mu{}^j{}_r(\varphi(x))\frac{\delta}{\delta\Gamma_\mu{}^j{}_s(\varphi(x))}+\frac{\partial_\mu\delta}{\delta\Gamma_\mu{}^r{}_s(\varphi(x))}\right\} \tag{2.11}$$

such that:

$$[D^s{}_r(x),D^l{}_m(y)]=f^s{}_r{}^l{}_m{}^j{}_i D^i{}_j(x)\delta(x-y) = (-\delta^s{}_m\delta^i{}_r\delta^l{}_j+\delta^l{}_r\delta^i{}_m\delta^s{}_j) \times D^i{}_j(x)\delta(x-y). \tag{2.12}$$

If we introduce the anticommuting Fadeev–Popov ($\Phi\Pi$) charged ghosts $C^i{}_j(x)$,

$$\{C^i{}_j(x),C^r{}_s(x)\}_+=0, \tag{2.13}$$

then we can define the BRS operator δ,

$$\delta=\int d^d x\left[C^i{}_j(x)D^j{}_i(x) - \frac{1}{2}f^s{}_r{}^l{}_m{}^i{}_j C^r{}_s(x)C^m{}_l(x)\frac{\delta}{\delta C^i{}_j(x)}\right] \tag{2.14}$$

$$=\int d^d x\left[C^i{}_j(x)D^j{}_i(x)+C^r{}_s(x)C^s{}_l(x)\frac{\delta}{\delta C^r{}_l(x)}\right], \tag{2.15}$$

such that

$$\delta^2=0.$$

Our program is now to investigate the cohomology space of the operator δ in order to find the local anomalies whose presence prevents the renormalization of the model.

Obviously, due to the nonlinearity of the model, the cohomology spaces must contain nonpolynomial objects too, so, many of the simplifications occurring in the polynomial quantum field theory (such as dimensional bounds) are not available.

On the other hand, some help can be obtained by the superselection rules of the model; first of all, in order to have objects with definite $\Phi\Pi$ charge, and to preserve the $\Phi\Pi$ charge additivity, we shall only consider functions which are analytical in the $\Phi\Pi$ ghosts and their derivatives; so if F is a local functional of the theory, to which corresponds a local function $F(x)$ in a space $\mathfrak{f}$, we decompose

$$F=\int d^d x\,F(x)=\int d^d x\,F_0(V,\Gamma)(x) + \int d^d x\sum_{n=1}(\partial_{\alpha(1)}\cdots\partial_{\alpha(n)}C^{i(1)}{}_{j(1)}(x))F_1{}^{j(1),\alpha(1)\cdots\alpha(n)}{}_{i(1)}(V,\Gamma)(x) + \int d^d x\sum_{n,m=1}(\partial_{\alpha(1)}\cdots\partial_{\alpha(n)}C^{i(1)}{}_{j(1)}(x))(\partial_{\beta(1)}\cdots\partial_{\beta(m)}C^{i(2)}{}_{j(2)}(x)) \times F_2{}^{j(1)j(2)\alpha(1)\cdots\alpha(n)}{}_{i(1),i(2)}{}^{\beta(1)\cdots\beta(m)}(V,\Gamma)(x)+\cdots, \tag{2.16}$$

where the functions

$F_1{}^{j(1),\alpha(1)\cdots\alpha(n)}{}_{i(1)}(V,\Gamma)(x)$,

$F_2{}^{j(1)j(2)\alpha(1)\cdots\alpha(n)}{}_{i(1),i(2)}{}^{\beta(1)\cdots\beta(m)}(V,\Gamma)(x),\cdots$

are, in general, nonpolynomials in $V^a{}_b{}^i{}_k(\varphi(x))$ and $\Gamma_\mu{}^i{}_j(\varphi(x))$ and other possible $\Phi\Pi$ neutral quantities.

In short the functional F admits the decomposition

$$F=\int d^d x \sum_{m=0} F^m(x)=\int \sum_{m=0} F^m{}_d(x),$$

where the upper index denotes the ΦΠ charge eigenvalue, and the lower one the usual grading in the space of forms.

Now the cohomology equations

$$\delta F=0, \quad F\neq\delta F^* \quad \text{for arbitrary } F^*$$

are solved, at the level of local functions, by the system

$$\delta F^m{}_d(x)+\mathbf{d}F^{m+1}{}_{d-1}(x)=0, \tag{2.17}$$

$$F^m{}_d(x)\neq\delta F^{m-1}{}_d(x)+\mathbf{d}F^m{}_{d-1}{}^*(x), \tag{2.18}$$

where $\mathbf{d}$ is the exterior differential operator, and, if the base space is isomorphic to $\mathbf{R}^n$ (so the Poincaré Lemma can be used) we get the chain of equations

$$\begin{aligned}&\delta F^{m+1}{}_{d-1}(x)+\mathbf{d}F^{m+2}{}_{d-2}(x)=0,\\ &\delta F^{m+2}{}_{d-2}(x)+\mathbf{d}F^{m+3}{}_{d-3}(x)=0,\\ &\quad\vdots\\ &\delta F^{m+d}{}_0(x)=0.\end{aligned} \tag{2.19}$$

In the next section we shall solve the equation

$$\delta F^r{}_s(x)=0, \tag{2.20}$$

for any r and s, using the spectral sequences technique.

III. SPECTRAL SEQUENCES AND LOCAL ANOMALIES

In this section we discuss the equation

$$\delta F^r{}_s(x)=0, \tag{3.1}$$

and we shall find the cohomology class of the operator δ in the space of local functions.

The analysis is based on the spectral sequences technique, already used[4–6] in the study of QFT anomalies.

Indeed, the assumption, needed to preserve the ΦΠ charge additivity, that all the local functions of the theory are analytic in the ghost fields and their space-time derivatives, implies that the operator

$$\nu=\sum_{n=0}(1+n)D_{\alpha(n)}C^i{}_j(x)\frac{\delta}{\delta D_{\alpha(n)}C^i{}_j(x)} \tag{3.2}$$

[where $D_{\alpha(n)}C^i{}_j(x)=(\partial_{\alpha(1)}\cdots\partial_{\alpha(n)}C^i{}_j(x))$] will induce a grading on the space $\mathfrak{f}$ with integer eigenvalues, such that

$$\mathfrak{f}=\sum_{k\geq 0}\mathfrak{f}(k), \tag{3.3}$$

and each element $f(k)$ of the spaces $\mathfrak{f}(k)$ is eigenvector of the operator ν with eigenvalue equal to k.

Now, if we define

$$K(p)=\sum_{k>p}\mathfrak{f}(k) \tag{3.4}$$

(the space of functions whose eigenvalue is greater than p), it is easy to derive

$$\mathfrak{f}=K(0)\supset K(1)\supset K(2)\supset\cdots\supset K(p)\supset\cdots\supset K(\infty)$$

and

$$\delta K(p)\subset K(p). \tag{3.5}$$

It is obvious that in our case that the filtration process completely exhausts the space $\mathfrak{f}$, that is,

$$K(\infty)=0 \tag{3.6}$$

or, more precisely,

$$\lim_{p\to\infty}K(0)/K(p)=K(0). \tag{3.7}$$

The operator δ will be graded with respect to ν as

$$[\nu,\delta]_-=\sum_{p\geq 1}p\delta(p) \tag{3.8}$$

and the particular expressions of the operators $\delta(p)$ are

$$\begin{aligned}\delta(1)=\sum_{n\geq 0}\Big[&C^r{}_s(x)\mathscr{D}^s{}_r(x)\\ &+D_{\alpha(n)}(C^r{}_s(x)C^s{}_l(x))\frac{\partial}{\partial D_{\alpha(n)}C^r{}_l(x)}\Big],\end{aligned} \tag{3.9}$$

where

$$\begin{aligned}\mathscr{D}^s{}_r(x)=\Big\{&-D_{\alpha(n)}V^a{}_b{}^j{}_r(\varphi(x))\frac{\partial}{\partial D_{\alpha(n)}V^a{}_b{}^j{}_s(\varphi(x))}\\ &+D_{\alpha(n)}V^a{}_b{}^s{}_j(\varphi(x))\frac{\partial}{\partial D_{\alpha(n)}V^a{}_b{}^r{}_j(\varphi(x))}\\ &-D_{\alpha(n)}\Gamma_\mu{}^s{}_j(\varphi(x))\frac{\partial}{\partial D_{\alpha(n)}\Gamma_\mu{}^r{}_j(\varphi(x))}\\ &+D_{\alpha(n)}\Gamma_\mu{}^j{}_r(\varphi(x))\frac{\partial}{\partial D_{\alpha(n)}\Gamma_\mu{}^j{}_s(\varphi(x))}\Big\},\end{aligned} \tag{3.10}$$

$$\begin{aligned}\delta(k+1)=&D_{\alpha(k)}C^r{}_s(x)\mathscr{D}^s{}_r\{k\}(x)\\ &+D_{\alpha(k-1)}\partial_\mu C^r{}_s(x)\frac{\partial}{\partial D_{\alpha(k-1)}\Gamma_\mu{}^r{}_s(\varphi(x))},\\ &k=1,2,\ldots,\end{aligned} \tag{3.11}$$

and we have defined

$$\begin{aligned}\mathscr{D}^s{}_r\{k\}(x)=\sum_{n\geq k}\frac{n!}{k!(n-k)!}\Big\{&-D_{\alpha(n-k)}V^a{}_b{}^j{}_r(\varphi(x))\frac{\partial}{\partial D_{\alpha(n)}V^a{}_b{}^j{}_s(\varphi(x))}\\ &+D_{\alpha(n-k)}V^a{}_b{}^s{}_j(\varphi(x))\frac{\partial}{\partial D_{\alpha(n)}V^a{}_b{}^r{}_j(\varphi(x))}-D_{\alpha(n-k)}\Gamma_\mu{}^s{}_j(\varphi(x))\frac{\partial}{\partial D_{\alpha(n)}\Gamma_\mu{}^r{}_j(\varphi(x))}\\ &+D_{\alpha(n-k)}\Gamma_\mu{}^j{}_r(\varphi(x))\frac{\partial}{\partial D_{\alpha(n)}\Gamma_\mu{}^j{}_s(\varphi(x))}\Big\}.\end{aligned} \tag{3.12}$$

Using now a procedure proposed by Dixon,[5] we introduce the notion of adjointness in the $\mathfrak{f}$ space, to have a Hilbert space structure, and we define

$$\delta^+(1)=\sum_{n>0}\left[\mathscr{D}^s{}_r{}^+(x)\frac{\partial}{\partial C^r{}_s(x)}+D_{\alpha(n)}C^r{}_l(x)\frac{\partial}{\partial D_{\alpha(n)}(C^r{}_s(x)C^s{}_l(x))}\right], \tag{3.13}$$

where

$$\mathscr{D}^s{}_r{}^+(x)=\left\{-D_{\alpha(n)}V^a{}_b{}^j{}_s(\varphi(x))\frac{\partial}{\partial D_{\alpha(n)}V^a{}_b{}^j{}_r(\varphi(x))}+D_{\alpha(n)}V^a{}_b{}^r{}_j(\varphi(x))\frac{\partial}{\partial D_{\alpha(n)}V^a{}_b{}^s{}_j(\varphi(x))}\right.$$
$$\left.-D_{\alpha(n)}\Gamma_\mu{}^r{}_j(\varphi(x))\frac{\partial}{\partial D_{\alpha(n)}\Gamma_\mu{}^s{}_j(\varphi(x))}+D_{\alpha(n)}\Gamma_\mu{}^j{}_s(\varphi(x))\frac{\partial}{\partial D_{\alpha(n)}\Gamma_\mu{}^j{}_r(\varphi(x))}\right\}, \tag{3.14}$$

$$\delta^+(k+1)=\mathscr{D}^s{}_r\{k\}^+(x)\frac{\partial}{\partial D_{\alpha(k)}C^r{}_s(x)}+D_{\alpha(k-1)}\Gamma_\mu{}^r{}_s(\varphi(x))\frac{\partial}{\partial D_{\alpha(k-1)}\partial_\mu C^r{}_s(x)},\quad k=1,2,..., \tag{3.15}$$

with

$$\mathscr{D}^s{}_r\{k\}^+(x)=\sum_{n\geq k}\frac{n!}{k!(n-k)!}\left\{-D_{\alpha(n)}V^a{}_b{}^j{}_s(\varphi(x))\frac{\partial}{\partial D_{\alpha(n-k)}V^a{}_b{}^j{}_r(\varphi(x))}\right.$$
$$+D_{\alpha(n)}V^a{}_b{}^r{}_j(\varphi(x))\frac{\partial}{\partial D_{\alpha(n-k)}V^a{}_b{}^s{}_j(\varphi(x))}-D_{\alpha(n)}\Gamma_\mu{}^r{}_j(\varphi(x))\frac{\partial}{\partial D_{\alpha(n-k)}\Gamma_\mu{}^s{}_j(\varphi(x))}$$
$$\left.+D_{\alpha(n)}\Gamma_\mu{}^j{}_s(\varphi(x))\frac{\partial}{\partial D_{\alpha(n-k)}\Gamma_\mu{}^j{}_r(\varphi(x))}\right\}. \tag{3.16}$$

The cohomology space of the operator δ, as shown in Ref. 6 for finite length filtrations, and extended in Appendix A to infinite ones, is isomorphic to the space of the solutions of the system

$$\delta(k)\Delta(x)=0,\quad \delta^+(k)\Delta(x)=0,\quad k=1,2,.... \tag{3.17}$$

The first step is to solve the system

$$\delta(1)\Delta(x)=0,\quad \delta^+(1)\Delta(x)=0. \tag{3.18}$$

Since $\delta(1)^2=0$, the above system will identify, due to the Hodge decomposition, the cohomology space of the operator $\delta(1)$, so the spectral sequences method can be directly applied to this case.

The result, analyzed in detail in Appendix B, is

$$\Delta(x)=T^*(C^r{}_s(x)_x,$$
$$T^1(V^a{}_b{}^j{}_t(\varphi(x)),D_{\alpha(n)}V^c{}_d{}^i{}_r(\varphi(x)),\Gamma_\mu{}^i{}_v(\varphi(x)),$$
$$D_{\alpha(m)}\Gamma_\nu{}^p{}_q(\varphi(x)),D_{\alpha(k)}C^r{}_s(x)), \tag{3.19}$$

where the quantities

$$T^*(C^r{}_s(x)) \tag{3.20}$$

and

$$T^1(V^a{}_b{}^j{}_t(\varphi(x)),D_{\alpha(n)}V^c{}_d{}^i{}_r(\varphi(x)),\Gamma_\mu{}^i{}_v(\varphi(x)),$$
$$D_{\alpha(m)}\Gamma_\nu{}^p{}_q(\varphi(x)),D_{\alpha(k)}C^r{}_s(x)) \tag{3.21}$$

are invariant under the global $\mathscr{F}$ transformation, and $T^*(C^r{}_s(x))$ depends only on underived ghosts fields, while

$$T^1(V^a{}_b{}^j{}_t(\varphi(x)),D_{\alpha(n)}V^c{}_d{}^i{}_r(\varphi(x)),\Gamma_\mu{}^i{}_v(\varphi(x)),$$
$$D_{\alpha(m)}\Gamma_\nu{}^p{}_q(\varphi(x)),D_{\alpha(k)}C^r{}_s(x))$$

is either $\Phi\Pi$ neutral or contains only space-time derivatives of the $C^r{}_s(x)$ fields.

Furthermore, the condition

$$\delta(k+1)\Delta(x)=0,\quad \delta^+(k+1)\Delta(x)=0,$$
$$k=1,2,..., \tag{3.22}$$

implies

$$\{\delta^+(k+1),\delta(k+1)\}\Delta(x)=0,\quad k=1,2,..., \tag{3.23}$$

which, after a little algebra, can be written

$$\left\{\mathfrak{D}^r{}_s\mathfrak{D}^r{}_s{}^+ + D_{\alpha(k-1)}\partial_\mu C^r{}_s(x)\right.$$
$$\left.\times\frac{\partial}{\partial D_{\alpha(k-1)}}\partial_\mu C^r{}_s(x)\right\}\Delta(x)=0, \tag{3.24}$$

where

$$\mathfrak{D}^s{}_r=[\mathfrak{D}^s{}_r\{k-l_\mu\}+D_{\alpha(k-1)}\Gamma_\mu{}^s{}_r(\varphi(x))]. \tag{3.25}$$

Now, thanks the Hilbert space structure we have introduced, we obtain the condition

$$\langle\mathfrak{D}^r{}_s{}^+\Delta(x)|\mathfrak{D}^r{}_s{}^+\Delta(x)\rangle$$
$$+\left\langle\frac{\partial}{\partial D_{\alpha(k-1)}\partial_\mu C^r{}_s(x)}\Delta(x)\right.$$
$$\left.\times\left|\frac{\partial}{\partial D_{\alpha(k-1)}\partial_\mu C^r{}_s(x)}\Delta(x)\right\rangle=0, \tag{3.26}$$

and the positivity of the norm implies

$$\mathfrak{D}^r{}_s{}^+\Delta(x)=0,$$
$$\frac{\partial}{\partial D_{\alpha(k-1)}\partial_\mu C^r{}_s(x)}\Delta(x)=0. \tag{3.27}$$

From the last equation we can easily derive, using the analyticity of the functions of the space $\mathfrak{f}$ in the $\Phi\Pi$ charged fields and their space-time derivatives, that $\Delta(x)$ is independent on the derivatives of the $C^r{}_s(x)$ fields.

Thus we arrive at the result

$$\Delta(x)=T^*(C^r{}_s(x)),T^1(V^a{}_b{}^j{}_t(\varphi(x)),$$
$$D_{\alpha(n)}V^c{}_d{}^i{}_r(\varphi(x)),\Gamma_\mu{}^i{}_v(\varphi(x)),D_{\alpha(m)}\Gamma_\nu{}^p{}_q(\varphi(x))) \tag{3.28}$$

with the subsidiary condition

$$\mathfrak{D}^r{}_s + T^1(V^a{}_b{}^j{}_t(\varphi(x)), D_{\alpha(n)} V^c{}_d{}^i{}_j(\varphi(x)), \Gamma_\mu{}^l{}_v(\varphi(x)),$$
$$D_{\alpha(m)} \Gamma_\nu{}^p{}_q(\varphi(x))) = 0. \quad (3.29)$$

We remark that the $\Phi\Pi$ character of the anomaly is fully contained in the term $T^*(C^r{}_s(x))$ and the term

$$T^1(V^a{}_b{}^j{}_t(\varphi(x)), D_{\alpha(n)} V^c{}_d{}^i{}_r(\varphi(x)), \Gamma_\mu{}^l{}_v(\varphi(x)),$$
$$D_{\alpha(m)} \Gamma_\nu{}^p{}_q(\varphi(x)))$$

represents the anomaly in the $\Phi\Pi$ charge zero sector, and we shall call it $\Delta^0(x)$, so Eq. (3.28) can be written

$$\Delta(x) = T^*(C^r{}_s(x))\Delta^0(x). \quad (3.30)$$

We show now that $\Phi\Pi$ evenly charged local anomalies can be discarded.

Let us consider, as an example, the case in which the $\Phi\Pi$ charge is equal to 4 (it will be obvious now the argument can be extended to the general case),

$$\Delta(x) = (aC^r{}_s(x)C^s{}_t(x)C^t{}_l(x)C^l{}_r(x) + bC^s{}_s(x)C^r{}_t(x)C^t{}_l(x)C^l{}_r(x))\Delta^0(x). \quad (3.31)$$

Using anticommutativity, we derive

$$C^r{}_s(x)C^s{}_t(x)C^t{}_l(x)C^l{}_r(x) = -C^l{}_r(x)C^r{}_s(x)C^s{}_t(x)C^t{}_l(x) = 0, \quad (3.32)$$

so the first term drops out. Following now a method proposed by Bardeen and Zumino,[12] we introduce in the theory the quantity

$$H(x) = \ln(\det g_{ij}(\varphi(x))), \quad (3.33)$$

it is easy to derive that

$$\delta H(x) = C^s{}_s(x) \quad (3.34)$$

so

$$C^s{}_s(x)C^r{}_t(x)C^t{}_l(x)C^l{}_r(x)\Delta^0(x) = \delta[H(x)C^r{}_t(x)C^t{}_l(x)C^l{}_r(x)\Delta^0(x)], \quad (3.35)$$

which proves our statement.

It is obvious that the above argument also applies to the usual "trace"anomalies

$$\Delta(x) = C^r{}_r(x)\Delta^0(x). \quad (3.36)$$

IV. LOCAL FUNCTIONAL ANOMALIES

In this section we analyze the integrated anomalies in the sector with $\Phi\Pi$ charge 1, by solving, for low space-time dimensions, the system Eq. (2.19).

A. Two-dimensional case

We have to solve the system

$$\delta F^1{}_2(x) + \mathbf{d}F^2{}_1(x) = 0, \quad (4.1)$$
$$\delta F^2{}_1(x) + \mathbf{d}F^3{}_0(x) = 0, \quad (4.2)$$
$$\delta F^3{}_0(x) = 0, \quad (4.3)$$

where the zero-form $F^3{}_0(x)$ takes the expression

$$F^3{}_0(x) = C^r{}_t(x)C^t{}_l(x)C^l{}_r(x)\Delta^0{}_0(x) + \delta\Sigma^2{}_0(x) = C^l{}_r(x)\delta C^r{}_l(x)\Delta^0{}_0(x) + \delta\Sigma^2{}_0(x), \quad (4.4)$$

with arbitrary $\Sigma^2{}_0(x)$, and the neutral zero form $\Delta^0{}_0(x)$ satisfies

$$\delta\Delta^0{}_0(x) = 0. \quad (4.5)$$

Substituting we get

$$\delta F^2{}_1(x) + \mathbf{d}F^3{}_0(x) = \delta F^2{}_1(x) + 3\delta(C^l{}_r(x)\mathbf{d}C^r{}_l(x)\Delta^0{}_0(x)) + C^l{}_r(x)\delta C^r{}_l(x)d\Delta^0{}_0(x) + \mathbf{d}\delta\,\Sigma^2{}_0(x) = 0, \quad (4.6)$$

which requires

$$\mathbf{d}\Delta^0{}_0(x) = \delta\underline{\Delta}^0{}_0(x) \quad (4.7)$$

and $\underline{\Delta}^0{}_0(x)$ has $\Phi\Pi$ charge equal to -1.

Since this is forbidden in our model, the only remaining possibility is that

$$\mathbf{d}\Delta^0{}_0(x) = 0 \quad (4.8)$$

hence $\Delta^0{}_0(x)$ has to be a constant.

So, with an easy calculation we get

$$F^1{}_2(x) = a\Gamma_\mu{}^r{}_j(\varphi(x))\partial_\nu C^j{}_r(x)\mathbf{d}x^\mu \wedge \mathbf{d}x^\nu + \delta\Lambda^0{}_2(x) + d\Sigma^1{}_2(x), \quad (4.9)$$

since no cohomology element is contributed from Eqs. (4.1) and (4.2).

B. Three-dimensional case

Here we have to solve the system

$$\delta F^1{}_3(x) + \mathbf{d}F^2{}_2(x) = 0, \quad (4.10)$$
$$\delta F^2{}_2(x) + \mathbf{d}F^3{}_1(x) = 0, \quad (4.11)$$
$$\delta F^3{}_1(x) + \mathbf{d}F^4{}_0(x) = 0, \quad (4.12)$$
$$\delta F^4{}_0(x) = 0. \quad (4.13)$$

As shown in the previous section, the cocycle equation (4.13) gives no cohomology element, so the first contribution comes from the homogeneous solution of Eq. (4.12), giving

$$F^3{}_1(x) = C^r{}_t(x)C^t{}_l(x)C^l{}_r(x)\Delta^0{}_1(x) + \delta\Sigma^2{}_1(x) = C^l{}_r(x)\delta C^r{}_l(x)\Delta^0{}_1(x) + \delta\Sigma^2{}_1(x), \quad (4.14)$$

where, comparing with the two-dimensional case, only the lower form indices have been changed.

Proceeding as in the previous case, the term $\Delta^0{}_1(x)$ satisfies

$$\Delta^0{}_1(x) = d\underline{\Delta}^0{}_0(x) \quad (4.15)$$

with

$$\delta\underline{\Delta}^0{}_0(x) = 0,$$

so the anomaly takes the form

$$F^1{}_3(x) = \Gamma_\mu{}^r{}_j(\varphi(x))\partial_\nu C^j{}_r(x)\partial_\rho\underline{\Delta}^0{}_0(x)\mathbf{d}x^\rho \wedge \mathbf{d}x^\mu \wedge \mathbf{d}x^\nu + \delta\Lambda^0{}_3(x) + \mathbf{d}\Sigma^1{}_3(x), \quad (4.16)$$

which clearly reveals its two-dimensional origin.

C. Four-dimensional case

The system is now

$$\delta F^1{}_4(x) + \mathbf{d}F^2{}_3(x) = 0, \quad (4.17)$$

$$\delta F^2{}_3(x) + \mathbf{d}F^3{}_2(x) = 0, \tag{4.18}$$

$$\delta F^3{}_2(x) + \mathbf{d}F^4{}_1(x) = 0, \tag{4.19}$$

$$\delta F^4{}_1(x) + \mathbf{d}F^5{}_0(x) = 0, \tag{4.20}$$

$$\delta F^5{}_0(x) = 0. \tag{4.21}$$

The previous examples show that the only nontrivial contributions may come from the oddly ΦΠ charged cohomologies, so the term

$$\begin{aligned} F^5{}_0(x) &= C^r{}_s(x)C^s{}_t(x)C^t{}_l(x)C^l{}_m(x)C^m{}_r(x) \\ &\quad \times \Delta^0{}_0(x) + \delta\Sigma^4{}_0(x) \\ &= C^l{}_r(x)\delta C^r{}_s(x)\delta C^s{}_l(x)\Delta^0{}_0(x) + \delta\Sigma^4{}_0(x) \end{aligned} \tag{4.22}$$

will induce, by the same reasoning, terms in the system (4.17)–(4.21)

$$F^4{}_1(x) = 5\,\partial_\nu C^l{}_s(x)C^s{}_r(x)\delta C^r{}_l(x)\mathbf{d}x^\nu, \tag{4.23}$$

$$F^3{}_2(x) = 10\,\partial_\nu C^l{}_s(x)\partial_\mu C^s{}_r(x)C^r{}_l(x)\mathbf{d}x^\nu \wedge \mathbf{d}x^\mu, \tag{4.24}$$

$$F^2{}_3(x) = 10\,\partial_\nu C^l{}_s(x)\partial_\mu C^s{}_r(x)\Gamma_\rho{}^r{}_l(\varphi(x))\mathbf{d}x^\nu \wedge \mathbf{d}x^\mu \wedge \mathbf{d}x^\rho \tag{4.25}$$

(defined up to boundaries and total derivatives) and leads to an anomaly in the ΦΠ charged one-sector

$$\begin{aligned} F^1{}_4(x) &= 10\,\partial_\nu C^j{}_r(x)\{\Gamma_\mu{}^r{}_s(\varphi(x))\partial_\rho\Gamma_\sigma{}^s{}_j(\varphi(x)) \\ &\quad - \tfrac{1}{2}\Gamma_\mu{}^r{}_s(\varphi(x))\Gamma_\rho{}^s{}_l(\varphi(x))\Gamma_\sigma{}^l{}_r(\varphi(x))\} \\ &\quad \times \mathbf{d}x^\sigma \wedge \mathbf{d}x^\rho \wedge \mathbf{d}x^\mu \wedge \mathbf{d}x^\nu \\ &\quad + \delta\Lambda^0{}_4(x) + \mathbf{d}\Sigma^1{}_4(x), \end{aligned} \tag{4.26}$$

and the homogeneous solution of Eq. (4.19) will give a term

$$\begin{aligned} F^3{}_2(x) &= C^r{}_t(x)C^t{}_l(x)C^l{}_r(x)\Delta^0{}_2(x) + \delta\Sigma^2{}_2(x) \\ &= C^l{}_r(x)\delta C^r{}_l(x)\Delta^0{}_2(x) + \delta\Sigma^2{}_2(x) \end{aligned} \tag{4.27}$$

leading to an anomaly

$$\begin{aligned} F^1{}_4(x) &= \Gamma_\mu{}^r{}_j(\varphi(x))\partial_\nu C^j{}_r(x)\,\partial_\rho\Delta^0{}_1(x)\mathbf{d}x^\rho \wedge \mathbf{d}x^\mu \wedge \mathbf{d}x^\nu \\ &\quad + \delta\Lambda^0{}_4(x) + \mathbf{d}\Sigma^1{}_4(x), \end{aligned} \tag{4.28}$$

where the ΦΠ neutral one-form $\Delta^0{}_1(x)$ has to satisfy the constraint $\delta\Delta^0{}_1(x) = 0$.

A generalization of the outlined method to higher space-time dimensions leads to anomalies coming from the usual transgression of Chern classes.

Notice that in our treatment it is evident that in higher dimensions there are anomalies generated from lower dimensionality structures.

V. RIEMANNIAN ANOMALIES

In the preceding sections we have carried out the cohomological analysis of the anomalies, that is, the cohomology space of a well defined nilpotent operator δ has been found, and the solutions we have computed reflect all the local properties of this operator. Let us remark that the Riemannian character of the manifold is not contained in the operator δ, which describes only the infinitesimal variations of the model under diffeomorphisms.

In fact, a Riemannian structure is defined[13] by the existence of an inner product which induces a conjugate linear isomorphism between the connections of the vector bundle and its dual; so the connection is said to be Riemannian if

$$\Gamma_\rho{}^r{}_l(\varphi(x)) + \Gamma_\rho{}^l{}_r(\varphi(x)) = 0, \tag{5.1}$$

which leads to a curvature tensor

$$\begin{aligned} R^l{}_r(\varphi(x)) &= \{\partial_\rho\Gamma_\sigma{}^l{}_r(\varphi(x)) + \Gamma_\rho{}^l{}_s(\varphi(x))\Gamma_\sigma{}^s{}_r(\varphi(x))\} \\ &\quad \times dx^\rho \wedge dx^\sigma \end{aligned} \tag{5.2}$$

with the property

$$R^l{}_r(\varphi(x)) + R^r{}_l(\varphi(x)) = 0. \tag{5.3}$$

Now the above conditions hold locally in all the manifold; however, since the infinitesimal $\mathscr{F}$ transformation maps zero into zero, we have to satisfy

$$\delta[\Gamma_\rho{}^r{}_l(\varphi(x)) + \Gamma_\rho{}^l{}_r(\varphi(x))] = 0, \tag{5.4}$$

$$\delta[R^l{}_r(\varphi(x)) + R^r{}_l(\varphi(x))] = 0, \tag{5.5}$$

which are verified by

$$C^l{}_r(x) = -C^r{}_l(x), \tag{5.6}$$

and the $\mathscr{F}$ field's diffeomorphisms become local Lorentz transformations.

In this situation it is easy to verify that the symmetric polynomials $T^*(C^r{}_s(x))$, in Sec. III, will give contributions only if they have ΦΠ charge equal to $4k-1$ with k integer.

This implies that the term $F^5{}_0(x)$ we have encountered in the previous section becomes trivial, and the integrals of all the quantities of the system (4.17)–(4.21) (and in particular the four-dimensional anomaly) disappear.

On the other hand, all the solutions of the two-dimensional chain [Eqs. (4.1)–(4.3)] fully satisfy the above requirements, and so we evidentiate the existence of ΦΠ charged 1 anomalies in space-time dimensions equal to $4k-2$ with k integer.

Concerning the remaining three- and four-dimensional anomalies of Sec. IV, they will survive only if the terms $\Delta^0{}_0(x)$ and $\Delta^0{}_1(x)$ satisfy all the above constraints.

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APPENDIX A: INTRODUCTION TO SPECTRAL SEQUENCES

In this Appendix we give a brief introduction to the spectral sequences technique. For a more exhaustive treatment we refer the reader to Ref. 9.

Let K be a differential complex with differential operator δ; i.e., K is an Abelian group and δ: $K \Rightarrow K$ is a group homomorphism such that $\delta^2 = 0$.

Suppose that in K there is a grading $K = \Sigma_{k\in Z}\, C^k$ and δ: $C^k \Rightarrow C^{k+1}$ increases the grading by 1.

The infinite sequence of subcomplexes

$$\begin{aligned} K = K(0) \supset K(1) \supset K(2) \supset \cdots \supset K(p) \\ \supset K(p+1) \supset \cdots \supset K(\infty) = 0 \end{aligned} \tag{A1}$$

is called a filtration on K, this makes K into a filtered complex.

In our case the grading number is given by the eigenvalue of the ΦΠ ghosts and their space-time derivatives counting operator ν, so the space $K(p)$ contains elements whose eigenvalue is greater than p.

Suppose now that the filtration has the property

$$\delta K(p) \subset K(p) \quad \text{for all } p. \tag{A2}$$

The operator δ will be graded with respect to ν as

$$[\nu,\delta]_- = \sum_{p\geqslant 1} p\delta(p). \tag{A3}$$

Define now

$$\delta^{-1}K(p) = \{x \in \delta^{-1}K(p) \text{ if } \delta x \in K(p)\}, \tag{A4}$$

$$Z^p{}_r = K(p) \cap \delta^{-1}K(p+r) \quad \text{and} \quad Z^p{}_r = K(p) \text{ for } r<0, \tag{A5}$$

$$\delta Z^{p-r}{}_r = K(p) \cap \delta K(p-r). \tag{A6}$$

Now $Z^p{}_r$ contains $Z^{p+1}{}_{r-1}$ and $dZ^{p+1-r}{}_{r-1}$, so we can define

$$E^p{}_r = Z^p{}_r / \{Z^{p+1}{}_{r-1} + \delta Z^{p+1-r}{}_{r-1}\}, \tag{A7}$$

$$E_r = \sum_p E^p{}_r. \tag{A8}$$

It is evident that if $x \in K(p)$ and $\delta x = 0$ then $x \in E^p{}_r$ for all r, and if $x \in K(p)$ and $x = \delta y$, then x is not an element of $E^p{}_r$ for n large enough. Furthermore, δ maps $Z^p{}_r$ into $Z^{p+r}{}_r$ and $\{Z^{p+r}{}_{r-1} + \delta Z^{p+1-r}{}_{r-1}\}$ into $\delta Z^{p+r}{}_{r-1}$ and since

$$E^{p+r}{}_r = Z^{p+r}{}_r / \{Z^{p+1+r}{}_{r-1} + \delta Z^{p+1}{}_{r-1}\},$$

δ will induce a differential $d_r: E^p{}_r \Rightarrow E^{p+r}{}_r$ whose cohomology space can be computed as follows.

(1) The space $Z^p(E_r)$ of cycles in $E^p{}_r$ is defined by $x \in Z^p{}_r$ such that

$$\delta x \in \{Z^{p+1+r}{}_{r-1} + \delta Z^{p+1}{}_{r-1}\},$$

i.e., $\delta x = \delta y + z$, with

$$y \in Z^{p+1}{}_{r-1}, \quad z \in Z^{p+1+r}{}_{r-1},$$

now, if $x = y + u$, we get $\delta u = z$, i.e., $u \in \delta^{-1}Z^{p+1+r}{}_{r-1}$, or, better $u \in K(p) \cap \delta^{-1}K(p+r+1) = Z^p{}_{r+1}$, and, since $Z^{p+1}{}_{r-1}$ is in the "denominator" of $E^p{}_r$, we can get

$$\begin{aligned} Z^p(E_r) &= \{Z^p{}_{r+1} + Z^{p+1}{}_{r-1}\} \\ &\quad \times \{Z^{p+1}{}_{r-1} + \delta Z^{p+1-r}{}_{r-1}\}^{-1} \\ &= E^p{}_r \cap Z^p{}_{r+1}. \end{aligned} \tag{A9a}$$

(2) The space of coboundaries $B^p(E_r)$ in $E^p{}_r$ contains the elements $z \in \delta Z^{p-r}{}_r$, so

$$\begin{aligned} B^p(E_r) &= E^p{}_r \cap \delta Z^{p-r}{}_r = \{\delta Z^{p-r}{}_r + Z^{p+1}{}_{r-1}\} \\ &\quad \times \{Z^{p+1}{}_{r-1} + \delta Z^{p+1-r}{}_{r-1}\}^{-1}, \end{aligned} \tag{A9b}$$

and the cohomology space $H^p(E_r) = Z^p(E_r)/B^p(E_r)$ will have the form

$$\begin{aligned} H^p(E_r) &= \{E^p{}_r \cap Z^p{}_{r+1}\} / \{E^p{}_r \cap \delta Z^{p-r}{}_r\} \\ &= \{Z^p{}_{r+1} + Z^{p+1}{}_{r-1}\} / \{\delta Z^{p-r}{}_r + Z^{p+1}{}_{r-1}\} \\ &= Z^p{}_{r+1} / \{Z^p{}_{r+1} \cap \{\delta Z^{p-r}{}_r + Z^{p+1}{}_{r-1}\}\} \\ &= Z^p{}_{r+1} / \{\delta Z^{p-r}{}_r + Z^{p+1}{}_{r-1}\} = E^p{}_{r+1} \subset E^p{}_r, \end{aligned} \tag{A10}$$

since $\delta Z^{p-r}{}_r \subset Z^p{}_{r+1}$ and $Z^p{}_{r+1} \cap Z^{p+1}{}_{r-1} = Z^{p+1}{}_{r-1}$.

Now

$$\lim_{r\to\infty} Z^p{}_r = K(p) \cap \delta^{-1}K(\infty) = K(p) \cap \delta^{-1}0,$$

which represents the space of cocycles of $K(p)$,

$$\lim_{r\to\infty} \delta Z^{p-r}{}_r = K(p) \cap \delta K(-\infty) = K(p) \cap \delta K,$$

which represents the space of coboundary of $K(p)$, and

$$E_\infty = \lim_{r\to\infty} E_r = \lim_{r\to\infty} \sum_p E^p{}_r = \sum_p \frac{H_p(K)}{H_{p+1}(K)},$$

which represents the graded cohomology group.

So the cohomology is reached first by the nested succession (in the index r) of the spaces $E^p{}_r$ and then summing in p in the sense of set theory.

Suppose now that K admits another filtration

$$K = K'(\infty) \supset \cdots \supset K'(p) \supset K'(p-1) \supset \cdots \supset K'(0) \tag{A11}$$

and $K'(p) = 0$ for $p<0$, and that there exists a scalar product such that $K'(p)$ will be orthogonal to $K(q)$ for $p \neq q$.

In our case this is fulfilled if we use the same filtration as before and if $K'(p)$ contains elements whose eigenvalue is less than or equal to p, and we adopt the scalar product defined in Sec. III.

We can now prove the following theorem.

Theorem: If $x_p \in E^p{}_r$, then the same $x_p \in E^p{}_{r+1}$ if

$$\delta(r)x_p = 0, \tag{A12}$$

$$\delta^+(r)x_p = 0, \tag{A13}$$

where $\delta^+(r)$ is the adjoint of $\delta(r)$ derived by the adjointness operation induced by our scalar product.

Proof: If $x_p \in E^p{}_r$, from Eq. (A10) we shall get that the same $x_p \in E^p{}_{r+1}$ if we have the following.

(1) $x_p \in Z^p{}_{r+1}$, that is, $x_p \in \delta^{-1}K(p+r+1)$,

and this will imply

$$\langle \delta x_p | K'(p+r) \rangle = 0,$$

where $\langle \ | \ \rangle$ means scalar product. If we decompose δx_p and $K'(p+r)$ in their components belonging to different eigenspace of the operator ν, then Eq. (A12) immediately follows.

(2) x_p has to be orthogonal to all elements of the space $\delta Z^{p-r}{}_r$, that is,

$$\langle \delta^+ x_p | K(p-r) \rangle = 0.$$

Equation (A13) is easily derived after the decomposition of $\delta^+ x_p$ and $K(p-r)$ into their ν eigenspaces.

Recalling now the definition of the spaces E_r we can use the above theorem to prove the following.

Lemma: If $x \in E_r$, then the same $x \in E_{r+1}$ if

$$\delta(r)x = 0, \tag{A14}$$

$$\delta^+(r)x = 0, \tag{A15}$$

and the space E_∞ can be "formally" derived solving the above infinite system.

APPENDIX B: THE COHOMOLOGY SPACE OF THE OPERATOR $\delta(1)$

In this Appendix we will study the cohomology space of the operator

$$\delta(1)=\left[C^r{}_s(x)\mathscr{D}^s{}_r(x)+\sum_{n>0}D_{\alpha(n)}\times(C^r{}_s(x)C^s{}_l(x))\frac{\partial}{\partial D_{\alpha(n)}C^r{}_l(x)}\right], \tag{B1}$$

where

$$\begin{aligned}\mathscr{D}^s{}_r(x)=\sum_{n>0}\Big\{&-D_{\alpha(n)}V^a{}_b{}^j{}_r(\varphi(x))\frac{\partial}{\partial D_{\alpha(n)}V^a{}_b{}^j{}_s(\varphi(x))}\\&+D_{\alpha(n)}V^a{}_b{}^s{}_j(\varphi(x))\frac{\partial}{\partial D_{\alpha(n)}V^a{}_b{}^r{}_j(\varphi(x))}\\&-D_{\alpha(n)}\Gamma_\mu{}^s{}_j(\varphi(x))\frac{\partial}{\partial D_{\alpha(n)}\Gamma_\mu{}^r{}_j(\varphi(x))}\\&+D_{\alpha(n)}\Gamma_\mu{}^j{}_r(\varphi(x))\frac{\partial}{\partial D_{\alpha(n)}\Gamma_\mu{}^j{}_s(\varphi(x))}\Big\}\end{aligned} \tag{B2}$$

using the spectral sequences techniques.

We shall use as the filtering operator

$$\nu=C^i{}_j(x)\frac{\partial}{\partial C^i{}_j(x)}, \tag{B3}$$

which decomposes the operator $\delta(1)$ into

$$\delta^0(1)=\sum_{n>k>2}\left[\frac{n!}{k!(n-k)!}D_{\alpha(k)}C^r{}_s(x)\times D_{\alpha(n-k)}C^s{}_l(x)\frac{\partial}{\partial D_{\alpha(n)}C^r{}_l(x)}\right] \tag{B4}$$

and

$$\begin{aligned}\delta^1(1)=C^r{}_s(x)\Big\{&\mathscr{D}^s{}_r(x)+\sum_{n>0}D_{\alpha(n)}C^s{}_l(x)\\&\times\frac{\partial}{\partial D_{\alpha(n)}C^r{}_l(x)}\\&-D_{\alpha(n)}C^l{}_r(x)\frac{\partial}{\partial D_{\alpha(n)}C^l{}_s(x)}\Big\}\\&+\left[(C^r{}_s(x)C^s{}_l(x))\frac{\partial}{\partial C^r{}_l(x)}\right].\end{aligned} \tag{B5}$$

The cohomology is obtained solving the system

$$\delta^0(1)\Delta(x)=0, \tag{B6}$$

$$\delta^{0+}(1)\Delta(x)=0, \tag{B7}$$

$$\delta^1(1)\Delta(x)=0, \tag{B8}$$

$$\delta^{1+}(1)\Delta(x)=0, \tag{B9}$$

which implies

$$\{\delta^0(1),\delta^{0+}(1)\}\Delta(x)=0, \tag{B10}$$

and

$$\{\delta^1(1),\delta^{1+}(1)\}\Delta(x)=0. \tag{B11}$$

From Eq. (B11) we derive

$$\{[\mathscr{M}^s{}_r(x)+\tfrac{1}{2}d^s{}_r(x)][\mathscr{M}^r{}_s(x)+\tfrac{1}{2}d^r{}_s(x)]+\tfrac{1}{4}d^r{}_s(x)d^s{}_r(x)\}\Delta(x)=0,$$

that is, using the Hilbert space structure,

$$\mathscr{M}^s{}_r(x)\Delta(x)=0, \tag{B12}$$

$$d^s{}_r(x)\Delta(x)=0, \tag{B13}$$

where

$$\mathscr{M}^s{}_r(x)=\mathscr{D}^s{}_r(x)+\sum_{n>0}D_{\alpha(n)}C^s{}_l(x)\frac{\partial}{\partial D_{\alpha(n)}C^r{}_l(x)}-D_{\alpha(n)}C^l{}_r(x)\frac{\partial}{\partial D_{\alpha(n)}C^l{}_s(x)},$$

$$d^s{}_r(x)=\left[(C^s{}_l(x))\frac{\partial}{\partial C^r{}_l(x)}-(C^l{}_r(x))\frac{\partial}{\partial C^l{}_s(x)}\right], \tag{B14}$$

and we have used the relations

$$[\mathscr{M}^s{}_r(x),\mathscr{M}^m{}_l(x)]=\delta^m{}_r\mathscr{M}^s{}_l(x)-\delta^s{}_l\mathscr{M}^m{}_r(x), \tag{B15}$$

$$[d^s{}_r(x),d^m{}_l(x)]=\delta^m{}_r d^s{}_l(x)-\delta^s{}_l d^m{}_r(x), \tag{B16}$$

which reveals that $\mathscr{M}^s{}_r(x)$ and $d^s{}_r(x)$ are in the adjoint representation of our group, and $\Delta(x)$ is invariant under their action, so Eq. (3.19) immediately follows.

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Ideal-preserving Lorentzian connections

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Fibers of the exterior bundle over a Lorentzian manifold can be given the structure of a Clifford algebra. The minimal left ideals of this Clifford algebra may be interpreted as spinors. In order to better understand spinorial properties of the Kähler equation in a curved space-time, conditions for the Lorentzian connection to preserve these ideals are examined.

I. INTRODUCTION

In 1962 Kähler investigated the relationship between a certain equation for differential forms and the Dirac equation.[1] He showed how certain solutions to this equation (the Kähler equation) corresponded to Dirac solutions to the hydrogen atom problem. Kähler's equation involves a section of the exterior bundle over space-time (or inhomogeneous differential form) and such a field has 16 components. In Minkowski space the equation may be decoupled into four identical equations for certain four-component fields that correspond to spinors. Before assigning a physical interpretation, if any, to the extra degrees of freedom in the Kähler equation it is important to know in which geometries the equation will decouple in this way. Graf[2] first emphasized that on a general Lorentzian manifold Kähler's equation does not admit spinorial solutions; indeed he gave a necessary condition for the existence of such solutions. However, the geometrical implications of his condition were not transparent and the question of classifying space-times in which it may be satisfied was not pursued. We shall here give such a geometrical interpretation and show how integrability conditions restrict the algebraic type of the curvature tensor. In fact a parametrization of the most general Lorentzian metric in which this condition may be satisfied can be given. Despite the interest in determining when Graf's condition may be satisfied we shall argue that this condition is not in fact strictly necessary for the Kähler equation to admit a spinorial solution and that a weaker condition will suffice, although we are unable to classify those geometries in which this weaker condition may be satisfied.

II. THEORY

Throughout this paper we shall work on a four-dimensional Lorentzian manifold M, with metric g. If d denotes the exterior derivative and * the Hodge dual then the Kähler equation for a neutral field is

$$\not{d}\phi = m\phi, \tag{1}$$

where $\not{d} = d - *d*$. Here ϕ is a section of the exterior bundle (or inhomogeneous differential form). The space of differential forms may be made into a Clifford algebra with the product $\vee$ defined by associativity and

$$A \vee \phi = A \wedge \phi + i_{\tilde{A}}\phi, \tag{2}$$

for A a one-form and ϕ any element. The g-adjoint to A is the tangent vector $\tilde{A}$ defined by

$$g(\tilde{A},B) = A(B), \quad \forall B \in T_P M. \tag{3}$$

The $\wedge$ denotes the exterior product and $i_{\tilde{A}}$ is the interior derivative. From now on we shall omit the $\vee$, it being understood that juxtapositioning of forms denotes their Clifford product. If ∇ is the metric-compatible torsion-free Lorentzian connection then

$$\not{d} = e^a \nabla_{X_a}, \tag{4}$$

where the coframe $\{e^a\}$ is dual to $\{X_a\}$.

The real Clifford algebra associated with a four-dimensional Lorentzian space is $C_{3,1}(\mathbb{R})$, which is isomorphic to the algebra of all real matrices of order 4. The (four-dimensional) minimal left ideals may form representation modules for the spin group. Elements of these ideals correspond to what are known in the physics literature as Majorana spinors. If the identity in $C_{3,1}(\mathbb{R})$ is written as a sum of pairwise orthogonal primitive idempotents

$$1 = \sum_{i=1}^{4} P_i, \tag{5}$$

then any element of the algebra, ϕ say, may be written as a vector-space sum of elements in nonintersecting minimal left ideals

$$\phi = \sum_{i=1}^{4} \phi P_i = \sum_{i=1}^{4} \phi_i. \tag{6}$$

In Minkowski space we may choose the P_i parallel, $\nabla_X P_i = 0$. Then if ϕ is any solution to (1) so are the ϕ_i. However, on an arbitrary Lorentzian manifold there are no parallel primitives, in fact later we shall give a parametrization of the most general metric that gives rise to a set of parallel primitives. In a general curved space we cannot solve (1) subject to the constraint that ϕ lie in some minimal left ideal, that is, $\phi = \phi P$ for some primitive P. Of course we could modify (1) so that it always had spinorial solutions. We may define a spinor covariant derivative S_X that preserves minimal left ideals such that

$$e^a S_{X_a}\psi = m\psi, \tag{7}$$

with $\psi = \psi P$, corresponds to the curved space Majorana–Dirac equation.[3,4] We wish here, however, to examine conditions for spinorial solutions to (1).

Graf[2] gave the condition that ∇_X act as an endomorphism on the left ideal projected by P as

$$P\nabla_X P = 0, \quad \forall X. \tag{8}$$

Of course we can choose a particular form of P and see what constraint (8) puts on the connection. However, it is not

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clear that the failure of a particular P to satisfy (8) precludes the existence of another primitive (which must be related to P by an arbitrary inner automorphism) that does. Different primitives can project out the same ideal. For if P and P' are primitives such that $P = PP'$ then if $\phi = \phi P$ we have $\phi = \phi P'$. One can show that if P and P' are related in this way then if either satisfies (8) so does the other as befits the fact that (8) is the condition that ∇_X preserve the ideal. This freedom in the choice of primitive can be exploited by characterizing every minimal left ideal by a primitive in a canonical form such that (8) has a clear geometrical interpretation. This is essentially equivalent to the correspondence between minimal left ideals of $C_{3,1}(\mathbf{R})$ and isotropic two-planes that we now describe.

If an isotropic two-plane Σ has a basis $\{x,a\}$, where x is a null one-form orthogonal to the unit one-form a, then we may associate a minimal left ideal with Σ by defining

$$I(\Sigma) = C_{3,1}(\mathbf{R})x(1+a). \tag{9}$$

At first glance it might appear that the ideal depends on the choice of basis for Σ whereas in fact it only depends on the orientation of the basis. One can show that every minimal left ideal of $C_{3,1}(\mathbf{R})$ is associated with an oriented isotropic two-plane in this way.[5] For a given Σ every $\psi \in I(\Sigma)$ determines a Σ' with basis $\{x',a'\}$ by

$$x'\psi = 0, \quad a'\psi = \psi. \tag{10}$$

The spinor ψ is said to represent Σ' (with respect to Σ). Two spinors in the same ideal, ψ and ψ', represent the same plane if and only if $\psi' = f\psi$ for some function f.[5] The condition that ∇_X preserve some minimal left ideal can now be stated in the following way.

Theorem: The following are equivalent.

(I) ∇_X is an endomorphism on some minimal left ideal, $I(\Sigma)$ say.

(II) ∇_X is an endomorphism on the isotropic two-plane Σ.

(III) S_X is an endomorphism on the space of representative spinors for Σ.

Suppose that (II) is true. Then by metricity we must have

$$\nabla_X x = \lambda_X x, \quad \nabla_X a = \mu_X x, \quad \forall X, \tag{11}$$

where the functions λ_X and μ_X depend linearly on X. Then

$$\nabla_X I(\Sigma) = \nabla_X C_{3,1}(\mathbf{R})x(1+a) + C_{3,1}(\mathbf{R})\lambda_X x(1+a),$$

since x is null and hence $x^2 = 0$.

So

$$\nabla_X I(\Sigma) = \{\nabla_X C_{3,1}(\mathbf{R}) + \lambda_X C_{3,1}(\mathbf{R})\}x(1+a)$$

and $\nabla_X I(\Sigma) \subset I(\Sigma)$.

Thus (II) $\Rightarrow$ (I).

Let ψ represent Σ with respect to some arbitrary plane then

$$x\psi = 0, \quad a\psi = \psi. \tag{12}$$

Differentiating this with S_X and using (11) gives

$$xS_X\psi = 0, \quad aS_X\psi = S_X\psi. \tag{13}$$

Thus $S_X\psi$ represents Σ, and since the space of representative spinors is one dimensional we must have

$$S_X\psi = \lambda'_x\psi, \tag{14}$$

and (II) $\Rightarrow$ (III).

Suppose now that (III) is true. Then differentiating (12) gives

$$\nabla_X x\psi = 0, \quad \nabla_X a\psi = 0. \tag{15}$$

Any one-form that annihilates ψ by left multiplication must be proportional to x. That is, (15) implies (11) and so (III) $\Rightarrow$ (II). We have already shown that (II) $\Rightarrow$ (I) and so (III) $\Rightarrow$ (I).

If (I) is true then we must have

$$\nabla_X\{x(1+a)\} = B_X x(1+a),$$

for some element B_X. Since ∇_X preserves the degree of forms the right-hand side of this expression is a sum of a one-form and a two-form. So B_X can always be taken to be a zero-form. (If this seems unreasonable then write B in a standard basis.) Thus if (I) is true we must have

$$\nabla_X x = \lambda_X x \quad \text{and} \quad \nabla_X(xa) = \lambda_X xa,$$

i.e.,

$$x\nabla_X a = 0 \quad \text{or} \quad \nabla_X a = \mu_X x.$$

So (I) $\Rightarrow$ (II) and hence (I) $\Rightarrow$ (III).

A theorem due to Walker[6] gives a parametrization for the most general metric such that (II), and hence (I), is true. In a chart $\{u,v,y,z\}$ we may take the orthonormal coframes to be

$$\begin{aligned} &e^0 = e^f dv + e^{-f} du, \quad e^1 = e^{-f} du, \\ &e^2 = A\, dy + F\, dv, \quad e^3 = B\, dz + G\, dv, \end{aligned} \tag{16}$$

with A and F functions of y and v, B and G functions of z and v, and f an arbitrary function. The recurrent null one-form whose direction is preserved by the connection is dv. Given a metric it is not clear whether or not it can be parametrized as in (16) and so it is useful to look at the algebraic conditions on the curvature that are integrability conditions for (II). If $\{x,a\}$ is a basis for the preserved isotropic plane Σ then it is convenient to choose a coframe $\{x,a,y,b\}$, where y is a null one-form orthogonal to a such that $xy + yx = 1$. The one-form b is of unit norm and orthogonal to the other basis vectors. If the connection preserves Σ then we must have

$$\begin{aligned} &\nabla_X x = \lambda_X x, \quad \nabla_X a = \mu_X x, \\ &\nabla_X b = \alpha_X x, \quad \nabla_X y = \lambda_X y - \tfrac{1}{2}\mu_X a - \tfrac{1}{2}\alpha_X b. \end{aligned} \tag{17}$$

The complex structure given by the Hodge map enables $\Lambda^2(M)$, the space of two-forms, to be complexified. The anti-double-dual part of the curvature tensor can then be regarded as a self-adjoint operator, with respect to a complex Euclidean inner product, on this complex three-dimensional space. The Jordan canonical form of this operator gives the Petrov classification.[7] The decomposable null two-form ax is an eigenvector of the curvature with vanishing eigenvalue. This makes the anti-self-dual curvature, R^-, algebraically special. The first possibility is that R^- could vanish. Type D is possible if the curvature scalar is not zero, where type III is possible only if it is. The general type II possibility reduces to type N if the curvature scalar is zero. The recurrent null vector forms one of the principal null directions.

The algebraic classification of the curvature is complet-

ed by determining the eigenvectors of the Ricci tensor regarded as an endomorphism on $\Lambda^1(M)$. When (17) is satisfied the eigenvalues are the curvature scalar and zero. The recurrent null one-from x is an eigenvector with the curvature scalar as eigenvalue. The number of independent eigenvectors for each eigenvalue depends on the parameters in the metric (16).

In the spaces we have discussed one can look for solutions to (1) subject to the constraint that the field lie in a minimal left ideal. We are not, however, guaranteed the existence of a set of idempotents that are parallel as in (5) and so cannot project an arbitrary solution to (1) into spinorial solutions. If we have a complete set of pairwise orthogonal parallel primitive idempotents then the connection preserves four nonintersecting minimal left ideals. In fact this latter condition is equivalent to the former. For if

$$1 = \sum_{i=1}^{4} P_i$$

and ∇_X preserves the ideals projected by the P_i then $\Sigma_{i=1}^4 \nabla_x P_i = 0$. If each term lies in one of the nonintersecting ideals then the sum can vanish ony if the terms vanish separately. If the algebra is a direct vector space sum of minimal left ideals,

$$C_{3,1}(\mathbb{R}) = \sum_{i=1}^{4} I(\Sigma_i), \tag{18}$$

then the Σ_i cannot all contain the same null one-form, for there is no null one-form that annihilates every element of the algebra by multiplication from the right. If Σ_1, say, is spanned by $\{x,a\}$ then if y is in Σ_2 such that y and x are linearly independent then we can scale y such that $xy + yx = 1$. Then since ∇_X preserves Σ_1 we must have (17), but if ∇_X also preserves Σ_2 then y is recurrent and thus we must have

$$\begin{aligned} &\nabla_X x = \lambda_X x, \quad \nabla_X y = -\lambda_X y, \\ &\nabla_X a = 0, \quad \nabla_X b = 0. \end{aligned} \tag{19}$$

As well as being necessary, Eqs. (19) are by inspection sufficient for ∇_x to preserve a set of nonintersecting minimal left ideals. When (19) is satisfied Walker's theorem[6] ensures that the metric can be cast in the form[8]

$$g = f^2(dx \otimes dx - dt \otimes dt) + dy \otimes dy + dz \otimes dz, \tag{20}$$

where f is a function of x and t. Such spaces are generically Petrov type D, and the only one that does not violate the dominant energy condition is flat space.

We have completely determined the spaces in which the connection acts as an endomorphism on some minimal left ideal. However, one should not conclude, as Graf [2] did, that such a geometry is necessary for the existence of a solution to the Kähler equation that lies in a minimal left ideal. For let $\psi \in I(\Sigma)$ such that

$$\psi x = 0, \quad \psi a = \psi. \tag{21}$$

Then there will be a null one-form that annihilates ψ by left multiplication. Generically this will not be x and we may choose it as y so that $xy + yx = 1$. If the coframe $\{x,y,a,b\}$ is dual to the frame $\{X,Y,A,B\}$ then

$$\not{d}\psi x = \not{d}(\psi x) - x\psi\nabla_X x - y\psi\nabla_Y x - a\psi\nabla_A x - b\psi\nabla_B x.$$

If we use (21) and $y\psi = 0$ then

$$\not{d}\psi x = -x\psi\nabla_X x - a\psi\nabla_A x - b\psi\nabla_B x.$$

Similarly

$$\not{d}\psi a = \not{d}\psi - x\psi\nabla_X x - a\psi\nabla_A x - b\psi\nabla_B x.$$

Thus if $\psi \in I(\Sigma)$ is a representative for a two-plane containing the null one-form y then $\not{d}\psi$ will be in $I(\Sigma)$ if and only if Σ is preserved under covariant differentiation with respect to vectors in the tangent three-plane determined by y. That is, we need

$$\nabla_V x = \lambda_V x, \quad \nabla_V a = \mu_V x, \quad \forall V\colon\ y(V) = 0. \tag{22}$$

The fact that $\not{d}\psi$ lies in the same ideal as ψ does not, of course, mean that we necessarily have a solution to (1). However, for the specific example of a gravitational plane wave we can find solutions to (1) that lie in an ideal characterized by a plane that satisfies (22), but not (17). (In this case there is in addition a different two-plane that is preserved by ∇_X for all X.) We cannot infer from (22) any restriction on the algebraic type of the curvature; indeed we have been unable to classify those spaces in which it can be satisfied.

III. COMMENTS

In this paper we have been concerned solely with minimal left ideals. Nonminimal ideals are also of interest. It is possible to put those nonminimal ideals of $C_{3,1}(\mathbb{R})$ that are projected out by primitives in the even subalgebra into correspondence with Dirac bispinors.[3] Such ideals are associated with null one-forms (rather than isotropic two-planes) and the methods of this paper are readily applied to the classification of geometries in which the connection preserves these ideals.

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KdV-invariant polynomial functionals

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It is proved that the algebra of the KdV-invariant polynomial functionals on the space of C^∞ functions on the one-dimensional torus is isomorphic to the polynomial algebra of the infinite number of the conserved quantities found by Miura, Gardner, and Kruskal [J. Math. Phys. **9**, 1204 (1968)]. As a corollary, it is shown that the algebra of the isospectral polynomial functionals of the Hill's operator also coincides with this algebra.

I. INTRODUCTION

It has been a while since the Korteweg–de Vries equation

$$u_t = uu_x + u_{xxx}$$

was recognized as a completely integrable Hamiltonian system, for example, on the space of C^∞ functions on the one-dimensional torus T^1. A complete set of its first integrals or invariants is provided[1] by the eigenvalues $\{\lambda_i[u]\}$ of the Hill's operator $-d^2/dx^2 + u(x)$, which are, however, highly transcendental functionals of u.

An infinite set of invariants $\{\tilde{I}_i[u]\}$ which are elementary functionals of u can be constructed through the asymptotic expansion

$$\sqrt{4\pi t}\sum_i \exp(-\lambda_i[u]t) \sim 1 + \sum_{i=1}^{\infty} \tilde{I}_i[u]t^i \quad (t\searrow 0).$$

In fact $\tilde{I}_i[u]$ is the integral of a local conserved density $I_i[u]$. Although the $I_i[u]$'s are known to exhaust the space of equivalence classes of the local conserved densities,[2] it is likely that these elementary invariants have less information than $\lambda_i[u]$'s and do not form a complete set of invariants of the KdV flow on the space of C^∞ functions on T^1. Note, however, that $I_i[u]$'s do have the same amount of information as $\lambda_i[u]$'s on the space of the real analytic functions on T^1 (Ref. 3).

In this paper, we take up the problem of whether or not there are other "elementary" invariants other than $\tilde{I}_i[u]$'s.

The functionals we consider as elementary are such $K[u]$'s as are expressible as

$$K[u] = \sum_n \int_{T^n} K_n(x_1,\ldots,x_n)u(x_1)\cdots u(x_n)dx_1\cdots dx_n ,$$

where K_n is a distribution on T^n and only a finite number of K_n's are nonzero. These will be called polynomial functionals. The space of the polynomial functionals is strictly larger than the space multiplicatively generated by those with local densities, since it includes those expressed as iterated integrals of local densities.

Our main result asserts that the functionals expressed as polynomials of $\tilde{I}_i[u]$'s are the only invariants that are polynomial functionals.

Our proof of this is rather involved due mainly to the simple topological fact that for $k\geqslant 3$ the space $\{(x_1,\ldots,x_k)\in T^k;\ x_i\neq x_j\ (i\neq j)\}$ is not connected. This fact gives rise to the possibility of the existence of first integrals expressible as iterated integrals of local conserved densities, which we were able to eliminate only after a detailed analysis of the local conserved densities of the KdV equation.

It seems to be an interesting problem to find a simpler proof, which admits us to infer whether other soliton equations have the same property or not.

For the evolution equations of space dimension greater than 1, it seems probable that the similar result can be rather easily established because the space $\{(x_1,\ldots,x_k)\in M^k;\ x_i\neq x_j\ (i\neq j)\}$ is connected for each k when $\dim M\geqslant 2$.

In Sec. II, we give basic definitions and state the main result (Theorem 2.3). The rest of the paper is devoted to its proof.

We start it first by describing the space of polynomial functionals by differential polynomials in Sec. III applying the idea of Gel'fand *et al.*[4] In Sec. IV, the derivation on the space of polynomial functionals corresponding to the KdV flow is expressed in terms of a derivation on the algebra of differential polynomials. The outline of the proof of the main result is exposed in Sec. V. Sections VI and VIII prove the key lemmas used in Sec. V and Sec. VII proves the algebraic independence of diagonal functionals.

In Sec. IX, we give several remarks and raise a few related problems.

We collected in the appendices certain facts and technical arguments in order to make it easier to see the main flow of the proof of the main result.

In Appendix A, we recall the structure theorem of distributions, with which we prove the propositions of Sec. VI. In Appendix B, we give basic definitions about differential polynomials and recall some of the basic facts in the theory of formal calculus of variation.[5] Appendix C recalls the result on the existence of an infinite number of independent conserved densities[6] and derives from it various consequences, which play crucial roles in various parts of our proof of the main result.

See Table I for a list of symbols used in the paper.

II. STATEMENTS OF THE MAIN RESULTS

A. Polynomial functionals

Let $T = \mathbf{R}/\mathbf{Z}$ be the one-dimensional torus and $F(T)$ the space of all the real valued C^∞ functions on T, which we

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TABLE I. List of symbols.

A:	the algebra of differential polynomials (Appendix B 1)
$\tilde{A}, A^i, A_n, A(d)$, etc.:	the subspaces of A defined in Appendix B 1
d:	the x derivation of A (Appendix B 1)
d_t:	the derivation of A corresponding to the KdV flow (Appendix C 1)
$\mathscr{D}'(X,Y)$:	the space of distributions on X with the supports in Y
δ_u:	the variational operator $A \to A$ (Appendix B 2)
Δ:	the endomorphism of A, the kernel of which is isomorphic to the space of the equivalence classes of local conserved densities of the KdV equation (Appendix C 1)
Δ^M:	a twisted version of Δ (Appendix C 4)
$F(T)$:	the space of real valued C^∞ functions on T
$F^k\mathscr{P}(F(T))$:	the Gelfand–Fuks filtration on $\mathscr{P}(F(T))$ (Sec. III B)
I_i:	the local conserved density of the KdV equation determined by Theorem C.7
$\tilde{I}_i$:	the local conserved quantity of the KdV equation, which is the integral of I_i
$\{\Omega,d\}$:	the complex associated to the KdV equation (Appendix C 1)
$\mathscr{P}(F(T))$:	the algebra of polynomial functionals on $F(T)$ (Sec. II A)
R:	the field of real numbers
S:	the symmetrization operator (Sec. III A)
$\mathfrak{S}_n$:	the permutation group
T:	the one-dimensional torus R/Z
T_i:	$= \delta_u I_i$ (Appendix C 2)
T_{ij}:	$= \delta_u(-I_iX_j + I_jX_i)$ (Appendix C 3)
$T^n(k)$:	$= \{(x_1,\ldots,x_n) \in T^n;\ \#\{x_1,\ldots,x_n\} \leqslant k\}$
X_i:	the flux for I_i determined by Theorem C.7
X_K:	the derivation of A corresponding to the evolutionary equation $u_t = K$ (Appendix B 3)
χ_k:	the map $\mathscr{D}'(T^k) \otimes \tilde{A}^{\otimes k} \to F^k\mathscr{P}(F(T))$ defined in Sec. III C
Z:	the ring of integers
Z_+:	the set of non-negative integers

All the vector spaces and all the tensor products are over R. For a group G and a G module V, the space of all the G-invariant elements is denoted by V^G.

identify with the periodic real valued C^∞ functions on R with period 1.

We call a real-valued functional $u \mapsto K[u]$ on $F(T)$ a *polynomial functional* if for $u \in F(T)$,

$$K[u] = K_0 + \sum_{n=1}^{\infty} \langle K_n, u^{\otimes n} \rangle , \tag{1}$$

where $K_0 \in \mathsf{R}$, $T^n = \mathsf{R}^n/\mathsf{Z}^n$, $K_n \in \mathscr{D}'(T^n) = \{$distributions on $T^n\}$, $u^{\otimes n} = u \otimes \cdots \otimes u$ (n times) is the C^∞ function on T^n defined by $u^{\otimes n}(x_1,\ldots,x_n) = u(x_1)\cdots u(x_n)$, and $K_n = 0$ except for finite n's.

Example 2.1: The following are some examples of polynomial functionals:

$$K_1[u] := u(x_0) ,$$

$$K_2[u] := \hat{u}(n) = \int_T e^{2\pi i n x} u(x)\, dx ,$$

$$K_3[u] := \int_T u(x) u'(x)^2\, dx ,$$

$$K_4[u] := \int_T u(x) u(x + x_0)\, dx ,$$

$$K_5[u] := \int_{0 \leqslant x_1 \leqslant \cdots \leqslant x_n \leqslant 1} f_1[u](x_1)\cdots f_n[u](x_n)\, dx_1 \cdots dx_n ,$$

where $x_0 \in T$, $f_i = f_i(u_0,u_1,\ldots)$ are differential polynomials (cf. Appendix A) and $f_i[u]$ denotes the function made by the substitutions: $u_i = d^i f/dx^i$.

The space of all the polynomial functionals is denoted by $\mathscr{P}(F(T))$, which is a commutative algebra by the multiplication:

$$K_1K_2[u] := K_1[u]K_2[u] , \quad u \in F(T) ,$$

for $K_1, K_2 \in \mathscr{P}(F(T))$.

A polynomial functional K is called *diagonal* or *local* if supp K_n is in the diagonal of T^n. For example, K_1, K_2, K_3, and K_5 with $n = 1$ are diagonal.

B. Spectral invariant functionals for the Hill operator

For $u \in F(T)$, we denote the spectrum of the Hill operator $L_u := -d^2/dx^2 + u$ by

$$\mathrm{Spec}(u) = \{\lambda_0 < \lambda_1 \leqslant \lambda_2 < \cdots < \lambda_{2i-1} \leqslant \lambda_{2i} < \cdots\} .$$

A real-valued functional K on $F(T)$ is called *spectral invar-*

iant if $\mathrm{Spec}(u)=\mathrm{Spec}(v)$ implies $K[u]=K[v]$ for $u,v\in F(T)$. We denote by $\mathscr{P}_{\mathrm{spec}}(F(T))$ the subalgebra of $\mathscr{P}(F(T))$ consisting of all the spectral-invariant polynomial functionals.

Example 1: For $u\in F(T)$ with $\mathrm{Spec}(u)=\{\lambda_i\}$, the following asymptotic expansion holds for $t\searrow 0$:

$$\sum_{i\geq 1}\exp(-\lambda_i t)\sim(4\pi t)^{-1/2}\left(1+\sum_{i\geq 1}\tilde{I}_i[u]t^i\right).$$

Moreover a universal differential polynomial I_i exists such that

$$\tilde{I}_i[u]=\int_0^1 I_i[u](x)dx\,.$$

Obviously the $\tilde{I}_i$'s are spectral invariant functionals, which are also polynomial and diagonal. Note that the differential polynomials I_i are not determined uniquely. We shall choose canonical ones by Theorem C.7.

C. KdV-invariant functionals

A functional K is called *invariant under the* KdV *flow*, or KdV *invariant* for short, if $K[u(\cdot,t)]$ is independent of t whenever $u(x,t)$ is a solution of the Korteweg–de Vries equation:

$$\frac{\partial u}{\partial t}=3u\frac{\partial u}{\partial x}-\frac{1}{2}\frac{\partial^3 u}{\partial x^3}\,. \tag{2}$$

We denote by $\mathscr{P}_{\mathrm{KdV}}(F(T))$ the subalgebra of $\mathscr{P}(F(T))$ consisting of all the KdV-invariant polynomial functionals.

The Lax representation of (2),

$$\frac{d}{dt}L_u=\left[2\frac{d^3}{dx^3}-\frac{3}{2}\left(u\frac{d}{dx}+\frac{d}{dx}u\right),L_u\right],$$

implies the following proposition.

Proposition 2.2: The spectral-invariant functionals are KdV invariant: $\mathscr{P}_{\mathrm{spec}}(F(T))\subset\mathscr{P}_{\mathrm{KdV}}(F(T))$.

D. Main theorem

Theorem 2.3: The algebra of the KdV-invariant polynomial functionals coincides with that of the spectral-invariant ones and is isomorphic to the polynomial algebra generated by $\tilde{I}_i$'s:

$$\mathscr{P}_{\mathrm{spec}}(F(T))=\mathscr{P}_{\mathrm{KdV}}(F(T))\cong\mathbf{R}[\tilde{I}_1,\tilde{I}_2,\ldots]\,.$$

This is an immediate consequence of Proposition 2.2 and the following theorem.

Theorem 2.4: The functionals $\tilde{I}_i$ are algebraically independent and generate the algebra of the KdV-invariant polynomial functionals.

We remark that the algebraic independence of the $\tilde{I}_i$'s has been already proved by Sunada.[7]

Remark: Our results imply that if a functional of iterated integral type such as K_5 in example 2.1 is spectral invariant, then there exists a unique polynomial $F(\tilde{I}_1,\ldots,\tilde{I}_N)$ with some N such that

$$K_5[u]=F(\tilde{I}_1[u],\ldots,\tilde{I}_N[u])\,,\quad u\in F(T)\,.$$

For example, Sunada[7] obtains such spectral invariants $A_i^n[u]$ as the coefficients in an asymptotic expansion:

$$\int_0^1 dx\int_\Omega\exp\left(-t\int_0^1 u(x+n\tau+\sqrt{t}\,\omega(\tau))d\tau\right)d\mu(\omega)$$
$$\sim 1+A_1^n[u]t+A_2^n[u]t^2+\cdots\quad(t\searrow 0)\,,$$

where Ω is the space of all the continuous functions ω: $[0,1]\to\mathbf{R}$ with $\omega(0)=\omega(1)$ and μ is the Wiener's measure on Ω. Our results imply that we can find polynomials $H_i^n\in\mathbf{R}[\tilde{I}_1,\tilde{I}_2,\ldots]$ such that

$$A_i^n[u]=H_i^n(\tilde{I}_1[u],\tilde{I}_2[u],\ldots)\,,\quad u\in F(T)\,.$$

This is a weaker version of the Sunada's result, which gives much more precise information about the polynomials H_i^n.

III. DESCRIPTION OF POLYNOMIAL FUNCTIONALS

Using a filtration similar to the one introduced by Gelfand *et al.*[4] in the computation of the continuous cohomology of the Lie algebra of vector fields, we describe the algebra of the polynomial functionals in terms of differential polynomials.

A. Identification of $\mathscr{P}(F(T))$ with the symmetric algebra of $\mathscr{D}'(T)$

A polynomial function on a vector space can be identified with an element of the symmetric algebra of its dual space. Analogously a polynomial functional K given by (1) can be identified with the sequence $(K_n)_{n=0,1,2,\ldots}$, where K_n is a symmetric distribution on T^n, i.e., $K_n^s=K_n$ for all $s\in\mathfrak{S}_n$, where $\langle K_n^s,f\rangle:=\langle K_n,{}^sf\rangle$ $(f\in F(T^n))$ with

$${}^sf(x_1,\ldots,x_n)=f(x_{s1},\ldots,x_{sn})\,.$$

Hereafter we make the following identification:

$$\mathscr{P}(F(T))=\bigoplus_{n=0}^{\infty}\mathscr{D}'(T^n)^{\mathfrak{S}_n},$$

where $\mathscr{D}'(T^n)^{\mathfrak{S}_n}$ denotes the space of the symmetric distributions on T^n.

Note that for $K\in\mathscr{D}'(T^n)$,

$$\langle K,u^{\otimes n}\rangle=\langle S(K),u^{\otimes n}\rangle\quad(u\in F(T))\,,$$

where $S(K)$ denotes the symmetrization of K:

$$S(K)=\frac{1}{n!}\sum_{s\in\mathfrak{S}_n}K^s\,.$$

B. Gelfand–Fuks filtration on $\mathscr{P}(F(T))$

For a subset X of T^n, denote by $\mathscr{D}'(T^n,X)$ the subspace of $\mathscr{D}'(T^n)$ consisting of all the distributions on T^n with supports in X. Define

$$T^n(k):=\{(x_1,\ldots,x_n)\in T^n;\ \#\{x_1,\ldots,x_n\}\leqslant k\}\,,$$

where $\#A$ stands for the number of the elements of a set A. Then $\mathscr{D}'(T^n,T^n(k))$ $(k=1,2,\ldots,n)$ is an $\mathfrak{S}_n$-invariant subspace of $\mathscr{D}'(T^n)$. We define $F^0\mathscr{P}(F(T))=\mathbf{R}$ and

$$F^k\mathscr{P}(F(T))=\bigoplus_{n\geq k}\mathscr{D}'(T^n,T^n(k)),\quad\text{for } k\geqslant 1\,.$$

This is an increasing filtration: $F^0\subset F^1\subset F^2\subset\cdots$, which is multiplicative, i.e., $F^pF^q\subset F^{p+q}$. Note that $F^1\mathscr{P}(F(T))$ is

exactly the space of the diagonal polynomial functionals. Note also, for example, that $K_4 \in F_2 \setminus F_1$ and $K_5 \in F_n \setminus F_{n-1}$ [cf. Example (2.1)].

C. Description of F^k/F^{k-1}

Let A be the algebra of differential polynomials of u (cf. Appendix B 1), and denote by $\tilde{A}$ the subspace of A consisting of all the elements with the zero constant terms: $\tilde{A} := \{f \in A; f(0) = 0\}$. Denote by $\tilde{A}^{\otimes k}$ the tensor product of k copies of $\tilde{A}$ over $\mathbb{R}$.

Define

$$\tilde{\chi}_k : \mathscr{D}'(T^k) \otimes \tilde{A}^{\otimes k} \to \mathscr{P}(F(T))$$

by

$$\tilde{\chi}_k(w \otimes f_1 \otimes \cdots \otimes f_k)[u] = \langle w, f_1[u] \otimes \cdots \otimes f_k[u] \rangle,$$

where $w \in \mathscr{D}'(T^k)$, $f_i \in \tilde{A}$, and $u \in F(T)$. This induces

$$\chi_k : [\mathscr{D}'(T^k) \otimes \tilde{A}^{\otimes k}]^{\mathfrak{S}_k} \to F_k \mathscr{P}(F(T)),$$

where $s \in \mathfrak{S}_k$ acts on $\mathscr{D}'(T^k) \otimes \tilde{A}^{\otimes k}$ by

$$s(w \otimes f_1 \otimes \cdots \otimes f_k) = w^s \otimes f_{t1} \otimes \cdots \otimes f_{tk}$$

$(t = s^{-1})$.

Then we have the following proposition.

Proposition 3.1: χ_k is surjective.

This will be proved in Appendix A using the structure theorems of distributions.

Now we describe $\chi_k^{-1} F_{k-1}$.

Define endomorphisms d_i $(i = 1,...,k)$ of $\mathscr{D}'(T^k) \otimes \tilde{A}^{\otimes k}$ by

$$d_i := \frac{\partial}{\partial x_i} \otimes 1 + 1 \otimes (1 \otimes \cdots \otimes 1 \otimes d \otimes 1 \otimes \cdots \otimes 1),$$

d being on the ith factor. Then we have the following proposition.

Proposition 3.2: $\chi_k^{-1}(F_{k-1}\mathscr{P}(F(T)))$ is spanned by

$$\left(\sum_{i=1}^{k} \operatorname{Im} d_i\right) \cap [\mathscr{D}'(T^k) \otimes \tilde{A}^{\otimes k}]^{\mathfrak{S}_k}$$

and

$$[\mathscr{D}'(T^k, T^k(k-1)) \otimes \tilde{A}^{\otimes k}]^{\mathfrak{S}_k}.$$

This will be also proved in Appendix A.

IV. THE KdV DERIVATION D_t ON $\mathscr{P}(F(T))$

We introduce a derivation D_t on $\mathscr{P}(F(T))$, which is in fact the infinitesimal generator of the KdV flow on $F(T)$ and $\operatorname{Ker} D_t = \mathscr{P}_{\mathrm{KdV}}(F(T))$ holds. In Sec. IV C, we find an operator which corresponds to D_t in the description of Sec. III C.

From now on, we rescale (x,t,u) to $(-x, 2t, -3u/2)$, so that the Korteweg–de Vries equation takes the simple form

$$\frac{\partial u}{\partial t} = u \frac{\partial u}{\partial x} + \frac{\partial^3 u}{\partial x^3}. \tag{3}$$

Observe that the validity of Theorem 2.4 does not change by this rescaling.

A. The infinitesimal generator of the KdV flow

To the KdV flow on $F(T)$ corresponds the derivation D_t on $\mathscr{P}(F(T))$ characterized by

$$\frac{d}{dt} K[u(\cdot,t)] = (D_t K)[u(\cdot,t)] \tag{4}$$

for $K \in \mathscr{P}(F(T))$ and all the solutions $u(x,t)$ of (3).

It is easy to see that this derivation can be expressed for $K \in \mathscr{D}'(T^n)^{\mathfrak{S}_n}$ as

$$D_t K = L_n + L_{n+1},$$

where

$$L_n = -nS\left(\frac{\partial^3}{\partial x_n^3} K_n(x_1,...,x_n)\right),$$

$$L_{n+1} = nS(K_n(x_1,...,x_n)\delta'(x_n - x_{n+1})).$$

Here $\delta(x-y) \in \mathscr{D}'(T^2)$ denotes the delta functional defined by

$$\langle \delta(x-y), f \rangle = \int_T f(x,x)\, dx, \quad f \in F(T^2),$$

and

$$\delta'(x-y) = \frac{\partial \delta(x-y)}{\partial x} = \frac{-\partial \delta(x-y)}{\partial y}.$$

B. Solvability of the Cauchy problem for the KdV equation

We recall the following theorem.

Theorem 4.1[3]**:** For every $u_0 \in F(T)$, a unique solution $u \in F(T \times \mathbb{R})$ of the KdV equation exists and satisfies $u(x,0) = u_0(x)$.

This implies the following proposition.

Proposition 4.2: $\mathscr{P}_{\mathrm{KdV}}(F(T)) = \operatorname{Ker} D_t$.

Proof: Obviously $D_t K = 0$ implies that K is KdV invariant by virtue of (4).

Conversely, let K be a KdV-invariant polynomial functional. For $u_0 \in F(T)$, let $u \in F(T \times \mathbb{R})$ be the solution of the KdV equation with $u(x,0) = u_0(x)$. Then by (4),

$$D_t K[u_0] = \frac{d}{dt} K[u(\cdot,t)] = 0.$$

Hence $D_t K = 0$. Q.E.D.

We note that the proof needs only solutions on $T \times (-\epsilon, \epsilon)$ with small positive ϵ.

We remark that we may as well define the notion of KdV invariance of a polynomial functional K by the technical condition $D_t K = 0$, which makes it unnecessary to rely on the above deep result.

C. Description of D_t in terms of differential polynomials

Define a derivation d_t of A by $d_t = X_{uu_1 + u_3}$ (cf. Appendix B 3), i.e.,

$$d_t := \sum_{i=0}^{\infty} d^i(uu_1 + u_3) \frac{\partial}{\partial u_i},$$

and endomorphisms $d_{t,i}$ $(i = 1,...,k)$ of $\mathscr{D}'(T^k) \otimes \tilde{A}^{\otimes K}$ by

$$d_{t,i} := 1 \otimes \cdots \otimes d_t \otimes \cdots \otimes 1,$$

d_t being in the ith place, and let

$$\tilde{d}_t := d_{t,1} + \cdots + d_{t,k}.$$

Then the following proposition holds.

Proposition 4.3: $D_t \circ \chi_k = \chi_k \circ \tilde{d}_t$.

Proof: For $f\in A$ and a solution u of (3) we have obviously

$$\frac{\partial f[u]}{\partial t}=(d_t f)[u]\,.$$

Using this, we have for $K\otimes f_1\otimes\cdots\otimes f_k\in\mathscr{D}'(T^k)\otimes\tilde{A}^{\otimes k}$

$$\begin{aligned}\frac{d}{dt}&(\tilde{\chi}_k(K\otimes f_1\otimes\cdots\otimes f_k)[u])\\&=\frac{d}{dt}\langle K,f_1[u]\otimes\cdots\otimes f_k[u]\rangle\\&=\sum_{i=1}^{k}\left\langle K,f_1[u]\otimes\cdots\otimes\frac{\partial f_i[u]}{\partial t}\otimes\cdots\otimes f_k[u]\right\rangle\\&=\tilde{\chi}_k(K\otimes\tilde{d}_t(f_1\otimes\cdots\otimes f_k))[u]\,.\end{aligned}$$

Hence, by Theorem 4.1, $D_t\circ\tilde{\chi}_k=\tilde{\chi}_k\circ\tilde{d}_t$, from which the proposition follows immediately. Q.E.D.

V. PROOF OF THE MAIN THEOREM 2.4

The algebraic independence follows from a general Theorem 7.1. So we prove in this section, $\mathscr{P}_{\mathrm{KdV}}(F(T))=\mathscr{P}_0$, where $\mathscr{P}_0$ denotes the subalgebra generated by $\tilde{I}_i$'s.

Let $K\in\mathscr{P}_{\mathrm{KdV}}(F(T))$. Let k be the integer satisfying

$$K\in F^k\mathscr{P}(F(T))\setminus F^{k-1}\mathscr{P}(F(T))\,.$$

We may suppose $k\geqslant 1$. We shall show that

$$K\in F^{k-1}\mathscr{P}(F(T))+\mathscr{P}_0\,.$$

Then by the induction on k it follows that $K\in\mathscr{P}_0$.

First by Proposition 3.1, K can be expressed as

$$K=\chi_k(J)$$

for some $J\in[\mathscr{D}'(T^k)\otimes\tilde{A}^{\otimes k}]^{\mathfrak{S}_k}$. Applying D_t to both sides, we obtain by Propositions 4.2 and 4.3

$$\chi_k(\tilde{d}_t J)=0\,.$$

Then Proposition 3.2 implies

$$\tilde{d}_t J\in\sum_{i=1}^{k}\operatorname{Im}d_i+\mathscr{D}'(T^k,T^k(k-1))\otimes\tilde{A}^{\otimes k}. \tag{5}$$

For each positive integer i, fix I_i and $X_i\in A$, which satisfies the conditions of Theorem C.7. Denote by C the subspace of A spanned by $\{I_i;\ i=1,2,3,\ldots\}$.

Define a subset T_0 of T^k by

$$T_0:=\{([x_1],\ldots,[x_k]);\ x_1<x_2<\cdots<x_k<x_1+1\}\,,$$

where $[x]\in\mathbb{R}/\mathbb{Z}$ denotes the class represented by $x\in\mathbb{R}$. Then obviously T_0 is a connected component of $T^k\setminus T^k(k-1)$. Let H be its characteristic function, i.e., H is 1 on T_0 and 0 on $T^k\setminus T_0$, which we regard as a distribution on T^k.

For $L\in\tilde{A}^{\otimes k}$ define

$$J_L:=\frac{1}{k!}\sum_{s\in\mathfrak{S}_k}s[H\otimes L]\in[\mathscr{D}'(T^k)\otimes\tilde{A}^{\otimes k}]^{\mathfrak{S}_k}.$$

Denote by $\mathfrak{F}_k$ the cyclic subgroup of $\mathfrak{S}_k$ generated by the cyclic permutation $(12\cdots k)$.

Lemma 5.1: If an element J of $[\mathscr{D}'(T^k)\otimes\tilde{A}^{\otimes k}]^{\mathfrak{S}_k}$ satisfies (5), then an $L\in[C^{\otimes k}]^{\mathfrak{F}_k}$ exists such that

$$\chi_k(J-J_L)\in F^{k-1}\mathscr{P}(F(T))\,.$$

This is, in fact, one of the two key points in our proof of the main theorem and will be proved in Sec. VI.

When $k\leqslant 2$, we have $J_L=1\otimes L$ because $T^k\setminus T^k(k-1)$ is connected. Hence we have mod $F^{k-1}\mathscr{P}(F(T))$,

$$K\equiv\chi_k(1\otimes L)\in\mathscr{P}_0\,,$$

which we wanted to show.

Suppose now $k\geqslant 3$.

We have proved that an $L\in[C^{\otimes k}]^{\mathfrak{F}_k}$ exists that satisfies

$$K-\chi_k(J_L)\in F^{k-1}\mathscr{P}(F(T))\,.$$

Then by Proposition 3.1 we have an $N\in[\mathscr{D}'(T^{k-1})\otimes\tilde{A}^{\otimes(k-1)}]^{\mathfrak{S}_{k-1}}$ satisfying

$$K=\chi_k(J_L)+\chi_{k-1}(N)\,.$$

Applying D_t, we obtain

$$D_t\chi_k(J_L)+\chi_{k-1}(\tilde{d}_t N)=0\,. \tag{6}$$

Now we calculate $D_t\chi_k(J_L)$. Define

$$\partial:\ C^{\otimes k}\to\tilde{A}^{\otimes(k-1)}$$

by

$$\begin{aligned}\partial(I_{i_1}\otimes\cdots\otimes I_{i_k})&=S(i_k,i_1)\otimes I_{i_2}\otimes\cdots\otimes I_{i_k}\\&\quad+\sum_{j=1}^{k-1}I_{i_1}\otimes\cdots\otimes I_{i_{j-1}}\otimes S(i_j,i_{j+1})\\&\quad\otimes I_{i_{j+2}}\otimes\cdots\otimes I_{i_k}\,.\end{aligned}$$

Here $S(i,j):=-I_iX_j+I_jX_i$. Then we have the following lemma.

Lemma: For $L\in C^{\otimes k}$,

$$D_t\chi_k(J_L)=\chi_{k-1}(J_{\partial L})\,.$$

Proof: For the sake of simplicity, we prove this when $k=3$. Let $L=Z(I_a\otimes I_b\otimes I_c)$. Then, for $u\in F(T)$,

$$\begin{aligned}(\chi_3 J_L)[u]=\int_0^1 dx\int_x^{x+1}dy\int_y^{x+1}dz\\\times I_a[u](x)I_b[u](y)I_c[u](z)\,.\end{aligned}$$

Let $f_i=I_i[u]$ and $g_i=X_i[u]$ $(i=a,b,c)$ for brevity. Since $d_tI_i=dX_i$, we have

$$(d_tI_i)[u]=(dX_i)[u]=g_i'\,.$$

Hence we have

$$\begin{aligned}D_t\chi_3(J_L)[u]&=\int_0^1 g_a'(x)\,dx\int_x^{x+1}f_b(y)\,dy\int_y^{x+1}f_c(z)\,dz+\int_0^1 f_a(x)\,dx\int_x^{x+1}g_b'(y)\,dy\int_y^{x+1}f_c(z)\,dz\\&\quad+\int_0^1 f_a(x)\,dx\int_x^{x+1}f_b(y)\,dy\int_y^{x+1}g_y'(z)\,dz\,.\end{aligned}$$

The first term is

$$\int_0^1 dx\left\{\left[g_a(x)\int_x^{x+1} f_b(y)\,dy\int_y^{x+1} f_c(z)\,dz\right]' + g_a(x)f_b(x)\int_x^{x+1} f_c(z)\,dz - g_a(x)\int_x^{x+1} f_b(y)\,dy f_c(x+1)\right\}$$
$$= \int_0^1 g_a(x)f_b(x)\,dx\int_x^{x+1} f_c(y)\,dy - \int_0^1 g_a(x)f_c(x)\,dx\int_x^{x+1} f_b(y)\,dy .$$

The second is

$$\int_0^1 f_a(x)dx\int_x^{x+1} dy\left\{\frac{\partial}{\partial y}\left[g_b(y)\int_y^{x+1} f_c(z)\,dz\right] + g_b(y)f_c(y)\right\}$$
$$= -\int_0^1 f_a(x)g_b(x)\int_x^{x+1} f_c(y)\,dy + \int_0^1 f_a(x)\,dx\int_x^{x+1} g_b(y)f_c(y)\,dy .$$

The third is

$$\int_0^1 f_a(x)\,g_c(x)\int_x^{x+1} f_b(y)\,dy - \int_0^1 f_a(x)\,dx\int_x^{x+1} f_b(y)g_c(y)\,dy .$$

Hence we have

$$D_t\chi_3(J_L)[u] = \int_0^1 (-f_a(x)g_b(x) + g_a(x)f_b(x))\,dx\int_x^{x+1} f_c(y)\,dy$$
$$+ \int_0^1 (-f_c(x)g_a(x) + g_c(x)f_a(x))\,dx\int_x^{x+1} f_b(y)\,dy$$
$$+ \int_0^1 f_a(x)\,dx\int_x^{x+1} (-f_b(y)g_c(y) + g_b(y)f_c(y))\,dy = \chi_2(J_{\partial L})[u] . \qquad \text{Q.E.D.}$$

By this lemma, (6) implies

$$\chi_{k-1}(J_{\partial L} + \tilde{d}_t N) = 0 . \tag{7}$$

Lemma 5.2: If an $L\in[C^{\otimes k}]^{\mathfrak{S}_k}$ satisfies (7) for an $N\in[\mathscr{D}'(T^{k-1})\otimes\tilde{A}^{\otimes(k-1)}]^{\mathfrak{S}_{k-1}}$, then L is $\mathfrak{S}_k$ invariant.

The proof of this is the most involved and will be given in Sec. VIII.

This lemma implies that $L\in[C^{\otimes k}]^{\mathfrak{S}_k}$, whence $J_L = 1\otimes L$. It follows then that mod $F^{k-1}\mathscr{P}(F(T))$

$$K\equiv\chi_k(1\otimes L)\in\mathscr{P}_0 .$$

This completes the proof of the main Theorem 2.4.

VI. PROOF OF LEMMA 5.1

We use the notations of Appendix B 4 with $M=\mathscr{D}'(T^k)$ and $\partial_j=\partial/\partial x_j$. Further, we define $\Delta_j := D_{K,j} + X_{K,j}$ with $K = uu_1 + u_3$.

Applying δ to the both sides of (5), we obtain

$$(\Delta_1 + \cdots + \Delta_k)\delta J\in\mathscr{D}'(T^k, T^k(k-1))\otimes\tilde{A}^{\otimes k} \tag{8}$$

because of Lemmas B.4 and B.5 and Corollary B.6.

Denote by r the restriction map from $\mathscr{D}'(T^k)\otimes\tilde{A}^{\otimes k}$ to $\mathscr{D}'(T^k\setminus T^k(k-1))\otimes\tilde{A}^{\otimes k}$. Then from (8) it follows

$$(\Delta_1' + \cdots + \Delta_k')r(\delta J) = 0 , \tag{9}$$

where Δ_i' $(i=1,\ldots,k)$ is the endomorphism of $\mathscr{D}'(T^k\setminus T^k(k-1))\otimes\tilde{A}^{\otimes k}$ denoted by Δ_i in Appendix B 4 for $M=\mathscr{D}'(T^k\setminus T^k(k-1))$ and $\partial_j=\partial/\partial x_j$.

Now we solve Eq. (9).

Let T_i be the variational derivative of I_i: $T_i=\delta_u I_i$ (cf. Appendix B 2 for the definition of δ_u). Denote by δC the subspace of $\tilde{A}$ spanned by the T_i's $(i=1,2,3,\ldots)$, and by LC(X), the space of locally constant real valued functions on a topological space X. Then the following lemma holds.

Lemma 6.1:

$$\mathrm{Ker}(\Delta_1' + \cdots + \Delta_k') = \mathrm{LC}(T^k\setminus T^k(k-1))\otimes(\delta C)^{\otimes k} .$$

Proof: We apply Lemma C.14 to $M=\mathscr{D}'(T^k\setminus T^k(k-1))\otimes\tilde{A}^{\otimes(k-1)}\otimes\mathsf{R}$ with $\partial=\partial/\partial x_k$ and $G=\Delta_1'+\cdots+\Delta_{k-1}'$. Then we obtain

$$\mathrm{Ker}(\Delta_1' + \cdots + \Delta_k')$$
$$= \left(\mathrm{Ker}\left(\frac{\partial}{\partial x_k}\right)\cap\mathrm{Ker}(\Delta_1' + \cdots + \Delta_{k-1}')\right)\otimes\delta C .$$

By induction, we obtain

$$\mathrm{Ker}(\Delta_1' + \cdots + \Delta_k')$$
$$= \left(\mathrm{Ker}\left(\frac{\partial}{\partial x_1}\right)\cap\cdots\cap\mathrm{Ker}\left(\frac{\partial}{\partial x_k}\right)\right)\otimes(\delta C)^{\otimes k} .$$

Q.E.D.

Hence we have

$$r(\delta J) = \sum_c H_c\otimes\delta(L_c) ,$$

where c ranges over the set of connected components of $T^k\setminus T^k(k-1)$, H_c is the characteristic function of c, and $L_c\in C$. Since J is $\mathfrak{S}_k$ symmetric, we have

$$\delta L_{sc} = \delta L_c$$

for all c and $s\in\mathfrak{S}_k$. Hence letting $L := L_{T_0}$, we have

$$r\delta(J - J_L) = 0 ,$$

which means

$$\delta(J - J_L)\in\mathscr{D}'(T^k, T^k(k-1))\otimes\tilde{A}^{\otimes k} .$$

It follows then by Lemma B.4 that

$$J-J_L\in\sum_{i=1}^{k}\operatorname{Im} d_i+\mathscr{D}'(T^k,T^k(k-1))\otimes\tilde{A}^{\otimes k},$$

whence by Proposition 3.2

$$\chi_k(J-J_L)\in F_{k-1}\mathscr{P}(F(T)).$$

Finally we note that L is $\mathfrak{S}_k$ invariant. In fact the $\mathfrak{S}_k$ invariance of T_0 implies that, for $s\in\mathfrak{S}_k$,

$$\delta(L-sL)=0,$$

whence $L=sL$ because of Lemma B.7. This completes the proof of Lemma 5.1.

VII. ALGEBRAIC INDEPENDENCE

We prove in this section the following theorem.

Theorem 7.1: Let $\{K_1,\dots,K_m\}$ be a linearly independent subset of $\bar{A}:=\chi_1(\mathrm{R}\otimes\tilde{A})\subset F^1\mathscr{P}(F(T))$. Then they are algebraically independent in the algebra $\mathscr{P}(F(T))$.

Proof: It suffices to show the injectivity of the map

$$a:\bigoplus_{k=0}^{\infty}[\bar{A}^{\otimes k}]^{\mathfrak{S}_k}\to\mathscr{P}(F(T))$$

induced by the multiplication. Moreover we have only to show for each k the injectivity of the map

$$a_k:\ [\bar{A}^{\otimes k}]^{\mathfrak{S}_k}\to F^k\mathscr{P}(F(T))/F^{k-1}\mathscr{P}(F(T))$$

induced from a, since

$$a([\bar{A}^{\otimes k}]^{\mathfrak{S}_k})\subset F^k\mathscr{P}(F(T)).$$

Suppose a_k is not injective, i.e.,

$$a(\bar{g})\in F^{k-1}\mathscr{P}(F(T)),$$

for some $\bar{g}\in[\bar{A}^{\otimes k}]^{\mathfrak{S}_k}$. Choose $g\in[Q^{\otimes k}]^{\mathfrak{S}_k}$ such that $\bar{g}=\chi_k(1\otimes g)$, where Q is a complement of $\operatorname{Im} d$ in $\tilde{A}$. Then by Proposition 3.2,

$$1\otimes g\in[\mathscr{D}'(T^k,T^k(k-1))\otimes\tilde{A}^{\otimes k}]^{\mathfrak{S}_k}+\sum_{i=1}^{k}\operatorname{Im} d_i.$$

Let T_0 be a connected component of $T^k\setminus T^k(k-1)$. Then on T_0 we have

$$1\otimes g\in\sum_{i=1}^{k}\operatorname{Im} d_i.$$

Now we use the results of Appendix B 4 with $M=\mathscr{D}'(T_0)$, $\partial_i=\partial/\partial x_i$. Then we have

$$\delta(1\otimes g)=0.$$

But this implies $\delta' g=0$, where δ' denotes the δ of Appendix B 4 with $M=R$ and $\partial_i=0$. By Lemma B.7, we have $g=0$, whence $\bar{g}=0$, establishing the injectivity of a_k. Q.E.D.

VIII. PROOF OF LEMMA 5.2

By virtue of Proposition 3.2, it suffices to prove the following. Let $Z=1/(k-1)!\,\Sigma_{s\in\mathfrak{S}_{k-1}}s$.

Lemma 8.1: Let $k\geqslant 3$. Suppose an

$$L=\sum a_{i_1\cdots i_k}I_{i_1}\otimes\cdots\otimes I_{i_k}\in[C^{\otimes k}]^{\mathfrak{S}_k}$$

satisfies

$$Z(\partial L)=\sum_{i=1}^{k-1}d_iN_i+\tilde{d}_tN\quad\text{on } T_0,\tag{10}$$

where T_0 is a component of $T^{k-1}\setminus T^{k-1}(k-2)$ and N_i, $N\in\mathscr{D}'(T_0)\otimes\tilde{A}^{\otimes(k-1)}$. Then $L\in[C^{\otimes k}]^{\mathfrak{S}_k}$.

Proof: Since L is $\mathfrak{S}_k$ invariant, we have

$$Z(\partial L)=\frac{k}{k-1}\sum_{j=1}^{k-1}a_{i_1\cdots i_k}I_{i_1}\otimes\cdots\otimes I_{i_{j-1}}\otimes S(i_j,i_{j+1})\otimes I_{i_{j+2}}\otimes\cdots\otimes I_{i_k}.$$

We use the notations of Appendix B 4 with $M=\mathscr{D}'(T_0)$ and $\partial_j=\partial/\partial x_j$. Let $\Delta_j=D_{K,j}+X_{K,j}$ with $K=uu_1+u_3$. Applying δ to (10) we obtain

$$\sum_{j=1}^{k-1}a_{i_1\cdots i_k}T_{i_1}\otimes\cdots\otimes T_{i_{j-1}}\otimes T_{ij_{j+1}}\otimes\cdots\otimes T_{i_k}=(\Delta_1+\cdots+\Delta_{k-1})P,\tag{11}$$

where $T_{ij}:=\delta(S(i,j))\in\tilde{A}$, $P=k/(k-1)\delta N$.

Sublemma 8.2: Let $k\geqslant 1$. The elements

$$\{T_{i_1}\otimes\cdots\otimes T_{i_{j-1}}\otimes T_{ij_{j+1}}\otimes\cdots\otimes T_{i_{k+1}};\ 1\leqslant j\leqslant k,\ i_a\in Z_+,\ i_j<i_{j+1}\}$$

are linearly independent in $\mathscr{D}'(T_0)\otimes\tilde{A}^{\otimes k}$ mod $\operatorname{Im}(\Delta_1+\cdots+\Delta_k)$.

By this, (11) implies

$$a_{ijj_3\cdots i_k}=a_{jii_3\cdots i_k}$$

for all $i,j,i_3,\dots,i_k$. Since $a_{i_1\cdots i_k}$ is cyclic with respect to the suffixes, it follows that $a_{i_1\cdots i_k}$ is actually symmetric, whence $L\in[C^{\otimes k}]^{\mathfrak{S}_k}$.

Thus it remains to prove Sublemma 8.2.

Let $k=1$. Suppose

$$\sum_{i<j}a_{ij}T_{ij}=\Delta P,\tag{12}$$

for some $P\in\mathscr{D}'(T)\otimes\tilde{A}$ with some $a_{ij}\neq 0$. We use the notations of Appendix C 4 with $M=\mathscr{D}'(T)$ and $\partial=\partial/\partial x$. Let P_i be the A^i_M component of P and put

$$m:=\max[\{2(i+j);\ a_{ij}\neq 0\}\cup\{i+3;\ \Delta P_i\neq 0\}].$$

Note that m must be even. In fact otherwise, we have $\Delta P_{m-3}=0$, contradicting to the definition of m.

Let $m=2s$. Then the A^{2s}_M component of (12) is

$$\sum_{i+j=s}a_{ij}T_{ij}=\Delta P_{2s-3}.$$

By applying Proposition C.12, we obtain $a_{ij}=0$ for $i+j=s$ and $P_{2s-3}=0$ contradicting to the definition of $m=2s$. Hence (12) implies $a_{ij}=0$ for all i and j.

Let now $k\geqslant 2$ and

$$\sum a^l_{i_1\cdots i_{l-1}sti_{l+1}\cdots i_k}T_{i_1}\otimes\cdots\otimes T_{i_{l-1}}\otimes T_{st}\otimes T_{i_{l+1}}\otimes\cdots\otimes T_{i_k}=(\Delta_1+\cdots+\Delta_k)P\tag{13}$$

with $P\in\mathscr{D}'(T_0)\otimes\tilde{A}^{\otimes k}$. Suppose some of the a's are nonzero. We use the notations of Appendix C 4 now with $M=\mathscr{D}'(T_0)\otimes\tilde{A}^{\otimes(k-1)}$ and $\partial=\partial/\partial x_k$. Then (13) can be rewritten as

$$a_i\otimes T_i+\sum_{i<j}a_{ij}\otimes T_{ij}=(G+\Delta^M)P,\tag{14}$$

where

$$a_{ij} := \sum a^{k}_{i_1\cdots i_{k-1}ij} \otimes T_{i_1} \otimes \cdots \otimes T_{i_{k-1}},$$

$$a_i := \sum_{l=1}^{k-1} a^{l}_{i_1\cdots i_{l-1}sti_{l+1}\cdots i_{k-1}i} T_{i_1} \otimes \cdots \otimes T_{i_{l-1}} \otimes T_{st} \otimes T_{i_{l+1}} \otimes \cdots \otimes T_{i_{k-1}},$$

$$G := \Delta_1 + \cdots + \Delta_{k-1}.$$

Let P_i be the A^{i}_{M} component of P. Let m be the maximum number in the union of $\{2(i+j);\ a_{ij}\neq 0\}$, $\{2i+2;\ a_i\neq 0\}$, and $\{i+3;\ (G+\Delta^M)P_i\neq 0\}$.

Suppose m is odd and let $m=2s+1$. Then the A^{2s+2}_{M} and A^{2s}_{M} components of (14) read

$$\Delta_3^M P_{2s-2} = 0,$$

$$\Delta_2^M P_{2s-2} + \Delta_3^M P_{2s-3} = \sum_{\substack{i<j \\ i+j=s}} a_{ij} \otimes T_{ij} + a_{s+1} \otimes T_{s+1}.$$

Then by virtue of Proposition C.12,

$$a_{s+1} + 3a_{1,s-1} = 0,$$

which implies $a_{s+1} = a_{1,s-1} = 0$ by virtue of Corollary C.9. Then by (ii) of Proposition C.12 $a_{ij}=0$ $(i+j=s)$ and $\Delta^M P_{2l-2}=0$, which contradicts the definition of m.

Let $m=2s$. Letting $P_{2s-2}=0$, we can use the above arguments to show that $a_s=0$, $a_{ij}=0$ $(i+j=s)$, and $\Delta_3^M P_{2s-3}=0$. But then $P_{2s-3}=0$ by Lemma C.11. We obtain again a contradiction.

This completes the proof of Sublemma 8.2 and hence that of Lemma 8.1. Q.E.D.

IX. REMARKS AND PROBLEMS[8]

(A) The validity of our result relies partly on the following algebraic fact: The map $\kappa: \wedge^2 H^1 \to H^2$ induced from the exterior product $\Omega^1\times\Omega^1\to\Omega^2$ (cf. Appendix C 1 for the notations) is injective, which is an easy consequence of Proposition C.12.

Problem: Are the similar maps for other soliton equations injective?

(B) Conversely if some evolution equation $u_t = F$ $(F\in\mathcal{A})$ has the nonzero kernel of $\wedge^2 H^1 \to H^2$, then we can construct an invariant that cannot be expressed as a polynomial of local conserved quantities. For example, suppose there are three one-forms $w_i = I_i\,dx + X_i\,dt$ $(i=1,2,3)$ such that $D_F w_i = 0$ $(i=1,2,3)$ and $w_1\wedge w_2 = D_F w_3$, i.e.,

$$d_t I_i = dX_i \quad (i=1,2,3),$$

$$I_1X_2 + I_2X_1 = dX_3 + d_tI_3,$$

where $d_t = X_F$ (cf. Appendix B 3). Then it is easily shown that

$$K[u] := \int_{-\infty}^{\infty} I_1(x_1)dx_1 \int_{-\infty}^{x_1} I_2(x_2)dx_2 + \int_{-\infty}^{\infty} I_3(x)dx$$

$[I_i(x) := I_i[u](x)]$ is an invariant with respect to the flow on the Schwarz space $\mathcal{S}(\mathsf{R})$ induced equation.

(C) A similar result as Theorem 2.4 can be obtained when we consider the KdV flow on the Schwarz space $\mathcal{S}(\mathsf{R})$ on R.

(D) When n is greater than 1, there are spectral invariant polynomial functionals for the Laplace operator $\Delta+u$ on the n-dimensional torus that cannot be expressed as a polynomial of local spectral invariants.[7]

Problem: Find all the spectral-invariant polynomial functionals: $F(T^n)\to\mathsf{R}$ for $-\Delta+u$ $(n\geqslant 2)$.

(E) We can consider a sort of de Rham complex on $F(T)$ as follows: A map $w: F(T)\times F(T)^p\to\mathsf{R}$ is called a *polynomial p-form* if it can be written as

$$w(u,X_1,\ldots,X_p) = \sum_N \int_{T^N\times T^p} w_N(x_1,\ldots,x_N;y_1,\ldots,y_p) \times u(x_1)\cdots u(x_N)X_1(y_1)\cdots X_p(y_p) \times dx_1\cdots dx_N\,dy_1\cdots dy_p$$

$[u,X_i\in F(T)]$, where w_N is a distribution on T^{N+p}, symmetric in the x_i's and antisymmetric in the y_i's, and where only a finite number of the w_N's are nonzero. Denote by $\Omega^pF(T)$ the space of all the polynomial p-forms. Define the exterior differentiation d: $\Omega^pF(T)\to\Omega^{p+1}F(T)$ by

$$dw(u,X_1,\ldots,X_{p+1}) = \sum_{N\geqslant 1}\sum_{i=1}^{p+1}(-1)^i \int_{T^{N-1}\times T^{p+1}} N \times w_N(x_1,\ldots,x_{N-1},y_i;y_1,\ldots,\hat{y}_i,\ldots,y_{p+1}) \times u(x_1)\cdots u(x_{N-1})X_1(y_1)\cdots X_{p+1}(y_{p+1}) \times dx_1\cdots dx_{N-1}\,dy_1\cdots dy_{p+1}.$$

Then we obtain a complex $\{\Omega^*F(T),d\}$. This is easily seen to be acyclic.

Let D_t be the Lie derivation on $\Omega^*F(T)$ induced by the KdV flow on $F(T)$. Since D_t commutes with d, we can define the subcomplex of invariant polynomial forms: $\Omega^*_{\mathrm{KdV}}F(T) := \mathrm{Ker}\,D_t$. Note that our main result asserts that $\Omega^0_{\mathrm{KdV}}F(T)\cong\mathsf{R}[\tilde{I}_1,\tilde{I}_2,\ldots]$.

Problem: Determine the space $\Omega^*_{\mathrm{KdV}}F(T)$ and then compute its cohomology.

The first step of the calculation goes just in the same way as in Secs. III and IV. The second step corresponding to the determination of the space of local conserved densities is to calculate the $E_1^{1,p}$ terms $(p\geqslant 1)$ of Vinogradov's spectral sequence[9,10] associated to the KdV equation, which does not seem to have been carried out yet.

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APPENDIX A: DISTRIBUTIONS

In this section, we recall structure theorems of distributions and prove Propositions 3.1 and 3.2.

1. Structure theorem of distributions

Let $\mathbf{R}^{n+m}=\mathbf{R}^n_x\times\mathbf{R}^m_y$ be the Euclidean space with the standard linear coordinate system $(x_1,\dots,x_n,y_1,\dots,y_m)$ and X the submanifold defined by $y_1=\cdots=y_m=0$, which we identify with $\mathbf{R}^n_x$. Let K be a compact subset of X.

Define

$$Q:\ \mathscr{D}'(\mathbf{R}^n_x,K)\otimes\mathbf{R}[\partial_x,\partial_y]\to\mathscr{D}'(\mathbf{R}^{n+m},K)$$

by

$$\langle Q(w\otimes\partial_x^A\partial_y^B),f\rangle=\langle w,\partial_x^A\partial_y^B f|_{y=0}\rangle\,,$$

for

$$w\in\mathscr{D}'(\mathbf{R}^n_x,K):=\{w\in\mathscr{D}'(\mathbf{R}^n_x)\ ;\ \mathrm{supp}(w)\subset K\}\,,$$

$$A\in\mathbf{Z}^m_+\,,\quad B\in\mathbf{Z}^n_+\,,$$

$$f\in F_0(\mathbf{R}^{n+m}):=\{\text{smooth functions on } \mathbf{R}^{n+m}\text{ with compact supports}\}.$$

Here $\partial_x=\partial/\partial x$, $\mathbf{R}[\partial_x,\partial_y]$ is the polynomial algebra on ∂_x and ∂_y, and ∂_x^A stands for $(\partial_{x_1})^{A_1}\cdots(\partial_{x_n})^{A_n}$ when $A=(A_1,\dots,A_n)$. The structure theorem of the distributions[11] can be formulated as the following theorem.

Theorem A.1: Q is an isomorphism on $\mathscr{D}'(\mathbf{R}^n_x,K)\otimes\mathbf{R}[\partial_y]$.

We describe now the kernel of Q: Define endomorphisms D_i $(i=1,\dots,n)$ of $\mathscr{D}'(\mathbf{R}^n_x,K)\otimes\mathbf{R}[\partial_x,\partial_y]$ by

$$D_i:=\partial_{x_i}\otimes 1+1\otimes\partial_{x_i}\,,$$

where ∂_{x_i} stands also for the multiplication map: $P(\partial_x,\partial_y)\mapsto P(\partial_x,\partial_y)\partial_{x_i}$. Then obviously Q maps $\mathrm{Im}\,D_1+\cdots+\mathrm{Im}\,D_n$ to zero. In fact we can show the following proposition.

Proposition A.2: (i) $\mathrm{Ker}\,Q=\Sigma_{i=1}^n\,\mathrm{Im}\,D_i$.

(ii) For a compact subset L of K,

$$Q^{-1}(\mathscr{D}'(\mathbf{R}^{n+m},L))=\mathscr{D}'(\mathbf{R}^n_x,L)\otimes\mathbf{R}[\partial_x,\partial_y]+\sum_{i=1}^n\mathrm{Im}\,D_i\,.$$

Proof: (ii) implies (i) if we put $L=\phi$. Suppose

$$Q\Big(\sum w_{AB}\otimes\partial_x^A\partial_y^B\Big)\in\mathscr{D}'(\mathbf{R}^{n+m},L)\,.$$

Since

$$w\otimes\partial_x^A\partial_y^B\equiv(-\partial_x)^A w\otimes\partial_y^B\quad\Big(\mathrm{mod}\sum_{i=1}^n\mathrm{Im}\,D_i\Big)\,,$$

we have

$$Q\Big(\sum(-\partial_x)^A w_{AB}\otimes\partial_y^B\Big)\in\mathscr{D}'(\mathbf{R}^{n+m},L)\,,$$

whence, by the above theorem,

$$\sum(-\partial_x)^A w_{AB}\otimes\partial_y^B\in\mathscr{D}'(\mathbf{R}^n,L)\otimes\mathbf{R}[\partial_y]\,.$$

Thus

$$\sum w_{AB}\otimes\partial_x^A\partial_y^B\in\mathscr{D}'(\mathbf{R}^n,L)\otimes\mathbf{R}[\partial_y]+\sum\mathrm{Im}\,D_i\,.\quad\text{Q.E.D.}$$

2. Decomposition of $\mathscr{D}'(T^n,T^n(k))$

We denote by $P(n,k)$ $(1\leqslant k\leqslant n)$ the set of all the partitions of $\{1,\dots,n\}$ into k nonvoid subsets:

$$P(n,k):=\{p=\{p_1,\dots,p_k\};\ p_1\cup\cdots\cup p_k=\{1,\dots,n\},\ p_i\neq\phi,\ p_i\cap p_j=\phi(i\neq j)\}\,.$$

For $p\in P$, let

$$T^n[p]:=\{(x_1,\dots,x_n)\in T^n;\ x_i=x_j\ \text{if}\ i,j\in p_a\ \text{for some}\ a\}\,.$$

Then

$$T^n(k)=\bigcup_{p\in P(n,k)}T^n[p]\,.$$

Since the subset T^n is regular in the sense of Schwarz,[11] we have the following lemma.

Lemma A.3: The map

$$g:\ \bigoplus_{p\in P(n,k)}\mathscr{D}'(T^n,T^n[p])\to\mathscr{D}'(T^n,T^n(k))$$

induced from the inclusions is surjective.

Denote by $\overline{P}(n,k)$ the subset of $P(n,k)$ consisting of all the p's satisfying the following condition: whenever $i<j$, $a\in p_i$, $b\in p_j$, one has $a<b$. Let $\mathfrak{S}_n$ act on $P(n,k)$ by

$$sp:=\{sp_1,\dots,sp_k\}\quad[s\in\mathfrak{S}_n,\ \ p\in P(n,k)]$$

and define for $p\in P(n,k)$ the subgroup

$$\mathfrak{S}(p):=\{s\in\mathfrak{S}_n;\ sp=p\}\,,$$

which leaves $\mathscr{D}'(T^n,T^n(p))$ invariant.

Lemma A.4: g induces a surjection:

$$g':=S\circ\bar{g}:\ \bigoplus_{p\in\overline{P}(n,k)}\mathscr{D}'(T^n,T^n[p])^{\mathfrak{S}(p)}\to\mathscr{D}'(T^n,T^n(k))^{\mathfrak{S}_n}\,,$$

where $\bar{g}$ is the restriction of g and S is the symmetrization.

Proof: Let $K\in\mathscr{D}'(T^n,T^n(k))^{\mathfrak{S}_n}$. By Lemma A.3,

$$K=\sum_{p\in P(n,k)}K_p$$

for some $K_p\in\mathscr{D}'(T^n,T^n[p])$. Then

$$K=\frac{1}{n!}\sum_{s\in\mathfrak{S}_n}sK=\frac{1}{n!}\sum_{p\in P(n,k)}\sum_{s\in\mathfrak{S}_n}sK_p=\frac{1}{n!}\sum_{q\in P(n,k)}\sum_{s\in\mathfrak{S}_n}sK_{s^{-1}q}\,.$$

Let

$$\tilde{K}_q:=\frac{1}{n!}\sum_{s\in\mathfrak{S}_n}sK_{s^{-1}q}\,.$$

Since $\mathrm{supp}(sK_p)\subset T^n[sp]$, we have $\tilde{K}_q\in\mathscr{D}'(T^n,T^n[q])$. Furthermore it is easy to see that $\tilde{K}_q$ is $\mathfrak{S}(q)$ invariant and that $s\tilde{K}_q=\tilde{K}_{sq}$. Hence noting that $\mathfrak{S}_n\overline{P}(n,k)=P(n,k)$, we obtain

$$K=\sum_{q\in P(n,k)}\tilde{K}_q=\sum_{p\in\overline{P}(n,k)}\frac{1}{m(p)!}\sum_{s\in\mathfrak{S}_n}s\tilde{K}_p=S\Big(\sum_{p\in\overline{P}(n,k)}\frac{n!}{m(p)!}\tilde{K}_p\Big)\,,$$

where $m(p)=\#\mathfrak{S}(p)$. Q.E.D.

3. Description of $\mathscr{D}'(T^n,T^n[p])^{\mathfrak{S}(p)}$

Define for $p\in\overline{P}(n,k)$ the subspace $A\langle p\rangle$ of $A^{\otimes k}$ spanned by all such elements $f_1\otimes\cdots\otimes f_k$ as f_i is homogeneous of degree $^{\#}p_i$ $(i=1,...,k)$. Denote the restriction of $\tilde{\chi}_k$ on $\mathscr{D}'(T^k)\otimes A\langle p\rangle$ by $\tilde{\chi}_p$.

Lemma A.5:

(i) $\operatorname{Im}\tilde{\chi}_p = g'(\mathscr{D}'(T^n,T^n[p])^{\mathfrak{S}(p)})$,

(ii) $\operatorname{Ker}\tilde{\chi}_p = \mathscr{D}'(T^k)\otimes A\langle p\rangle\cap\sum_{i=1}^{k}\operatorname{Im} d_i$,

(iii) $\chi_p^{-1}(\mathscr{D}'(T^n,T^n(k-1)))$

$$= \mathscr{D}'(T^k,T^k(k-1))\otimes A\langle p\rangle + \sum_{i=1}^{k}\operatorname{Im} d_i .$$

Proof: (i) Obviously the elements of the left-hand side are in the right-hand side.

Denote by $\bar{p}_i$ the number of the elements of p_i and denote the coordinates of R^n as $(x_{11},...,x_{1\bar{p}_1},...,x_{k\bar{p}_k})$. Then $T^n[p]$ is the submanifold defined by the equations

$$x_{11}=\cdots=x_{1\bar{p}_1},...,x_{k1}=\cdots=x_{k\bar{p}_k} .$$

Hence, by Theorem A.1, for each $K\in\mathscr{D}'(T^n,T^n[p])$ we can find such an element $\Sigma K_B\otimes\partial_x^B$ of $\mathscr{D}'(T^k)\otimes\mathsf{R}[\partial_x]$ as

$$(g'K)[u] = \sum\langle K_B, L_{B,1}u\otimes\cdots\otimes L_{B,k}u\rangle$$

for $u\in F(T)$, where

$$L_{B,i}u := \partial_{x_{i1}}^{B_{i1}}u\cdots\partial_{x_{i\bar{p}_i}}^{B_{i\bar{p}_i}} \quad (1\leqslant i\leqslant k)$$

$[B=(B_{11},...,B_{1\bar{p}_1},...,B_{k1},...,B_{k\bar{p}_k})]$. If we let

$$f_B := u_{B_{11}}\cdots u_{B_{1\bar{p}_1}}\otimes\cdots\otimes u_{B_{k1}}\cdots u_{B_{k\bar{p}_k}}\in A\langle p\rangle ,$$

then

$$(g'K)[u] = \tilde{\chi}_k\Big(\sum K_B\otimes f_B\Big)[u] ,$$

which shows (i). The other assertions follow immediately from Proposition A.2. Q.E.D.

4. Proof of Propositions 3.1 and 3.2

Proposition 3.1 follows directly from Lemma A.4 and (i) of Lemma A.5.

Proof of Proposition 3.2: Let $K\in\mathscr{D}'(T^k)\otimes\tilde{A}^{\otimes k}$. Since

$$\tilde{A}^{\otimes k} = \bigoplus_{n\geqslant k} A(k,n)$$

with

$$A(k,n) := \bigoplus_{p\in\overline{P}(n,k)} A\langle p\rangle ,$$

we can write

$$K = \sum_{n\geqslant k}\sum_{p\in\overline{P}(n,k)} K_p$$

with $K_p\in\mathscr{D}'(T^k)\otimes A\langle p\rangle$. Suppose $\tilde{\chi}_k(k)\in F^{k-1}P(F(T))$. Since $\tilde{\chi}_k(A(k,n))\subset\mathscr{D}'(T^n)^{\mathfrak{S}_n}$, we have for each n,

$$\tilde{\chi}_k\Big(\sum_{p\in\overline{P}(n,k)} K_p\Big)\in\mathscr{D}'(T^n,T^n(k-1))^{\mathfrak{S}_n} .$$

Hence for each $p\in\overline{P}(n,k)$ we have

$$\tilde{\chi}_k(K_p) = L - \sum_{q\in\overline{P}(n,k),q\neq p}\tilde{\chi}_k(K_q)$$

with $L\in\mathscr{D}'(T^n,T^n(k-1))$. Since

$$\operatorname{supp}\tilde{\chi}_k(K_q)\subset\bigcup_{s\in\mathfrak{S}_n} T^n[sq] ,$$

it follows

$$\operatorname{supp}\tilde{\chi}_k(K_p)\subset T^n(k-1)\cup\bigcup_{(q,s)}(T^n[p]\cap T^n[sq]) ,$$

where $(q,s)\in\overline{P}(n,k)\times\mathfrak{S}_n$ satisfies the condition either that $q\neq p$ or that $q=p$ and $s\neq\mathrm{id}$. Since

$$T^n[p']\cap T^n[p'']\subset T^n(k-1)$$

for $p'\neq p''$, we obtain

$$\operatorname{supp}\tilde{\chi}_k(K_p)\subset T^n(k-1) .$$

Then by (iii) of Lemma A.5,

$$K_p\in\mathscr{D}'(T^k,T^k(k-1))\otimes A\langle p\rangle + \sum_{i=1}^{k}\operatorname{Im} d_i .$$

Hence we have proved

$$\tilde{\chi}_k^{-1}(F^{k-1}\mathscr{P}(F(T))) = \mathscr{D}'(T^k,T^k(k-1))\otimes\tilde{A}^{\otimes k} + \sum_{i=1}^{k}\operatorname{Im} d_i .$$

Restricting this to $[\mathscr{D}'(T^k)\otimes\tilde{A}^{\otimes k}]^{\mathfrak{S}_k}$, we obtain the proposition. Q.E.D.

APPENDIX B: DIFFERENTIAL POLYNOMIALS

1. The differential algebra A of differential polynomials

Let A denote the algebra of differential polynomials of u:

$$A := \mathsf{R}[u_0,u_1,u_2,...] = \bigcup_{k=1}^{\infty}\mathsf{R}[u_0,u_1,...,u_k]$$

endowed with the derivation d defined by $du_i = u_{i+1}$ $(i=0,1,2,...)$. We write often u_0 simply by u.

We define the weight and the degree of differential polynomials multiplicatively by $\operatorname{weight}(u_i)=i+2$ and $\operatorname{degr}(u_i)=1$. We let

$$A^i := \{f\in A;\ \operatorname{weight}(f)=i\} ,$$

$$A_n := \begin{cases}\mathsf{R}[u_0,u_1,...,u_n] & \text{for } n\geqslant 0,\\ \mathsf{R} & \text{for } n=-1,\end{cases}$$

$$A(d) := \{f\in A;\ \operatorname{degr}(f)=d\} ,$$

$$A^{(i)} := \sum_{j\leqslant i}A^j ,\quad A[d] := \sum_{c\geqslant d}A(c) ,$$

$$A^i(d) := A^i\cap A(d) ,\quad A_n^i := A^i\cap A_n ,$$

$$\tilde{A} := A[1] ,\quad \overline{A} := A/\operatorname{Im} d .$$

The following lemma is well known.

Lemma B.1: $\operatorname{Ker} d = \mathsf{R}$.

Proof: Suppose $g\in A_n\setminus A_{n-1}$ satisfies $dg=0$. Suppose $n\geqslant 0$. Then $\partial g/\partial u_n = \partial/\partial u_{n+1}(dg) = 0$, a contradiction. Hence we must have $n=-1$, i.e., $g\in\mathsf{R}$. Q.E.D.

2. The variational operator δ_u

Define $\delta_u: A\to A$ by

$$\delta_u := \sum_{i=0}(-d)^i\circ\frac{\partial}{\partial u_i} .$$

Then the following proposition is well known.

Proposition B.2: $\operatorname{Ker}\delta_u = \mathsf{R} + \operatorname{Im} d$.

Proof: From $[\partial/\partial u_{i+1}, d] = \partial/\partial u_i$, it follows immediately that $\delta_u \circ d = 0$.

Suppose $\delta_u g = 0$ for some $g \in A$. Then

$$\sum u_i \frac{\partial g}{\partial u_i} \equiv u\delta_u g = 0 \pmod{\operatorname{Im} d},$$

whence $\Sigma i g_i \in \operatorname{Im} d$, g_i being the $A(i)$ component of g. By the induction on the integer $n = \max\{n | g_n \neq 0\}$ we can show $g \equiv g_0 \pmod{\operatorname{Im} d}$. Q.E.D.

3. Evolutional derivation X_K

For $K \in A$, define a derivation of A by

$$X_K := \sum_{i=0}^{\infty} d^i K \frac{\partial}{\partial u_i},$$

which commutes with d. Define an endomorphism D_K of A by

$$D_K := \sum_{i=0}^{\infty} (-d)^i \circ \frac{\partial K}{\partial u_i}.$$

For example, if $K = uu_1 + u_3$, then

$$D_K := u_1 - d \circ u - d^3 = -d^3 - ud.$$

Lemma B.3: $\delta_u \circ X_K = (D_K + X_K) \circ \delta_u$.

Proof: First we show

$$g\delta_u\, d_K f \equiv g(D_K + X_K)\delta_u f \pmod{\operatorname{Im} d}$$

for $f, g \in A$. In fact, mod Im d,

$$\begin{aligned} g\delta_u X_K f &\equiv X_g X_K f = X_g \sum_i d^i K \frac{\partial f}{\partial u_i} \\ &= \sum_i d^i \left(\sum_j d^j g \frac{\partial K}{\partial u_j} \right) \frac{\partial f}{\partial u_i} + \sum_{i,j} d^i K\, d^j g\, \frac{\partial^2 f}{\partial u_i\, \partial u_j} \\ &\equiv \sum_j d^j g \frac{\partial K}{\partial u_j} \delta_u f + \sum_j d^j g X_K \frac{\partial f}{\partial u_j} \\ &\equiv g\left(\sum_j (-d)^j \left(\frac{\partial K}{\partial u_j} \delta_u f \right) + \sum_j (-d)^j \left(X_K \frac{\partial f}{\partial u_j} \right) \right) \\ &= g(D_K \delta_u f + X_K \delta_u f). \end{aligned}$$

Now it is not difficult to see that, if $f \in A$ satisfies $fg \in \operatorname{Im} d$ for all $g \in A$, then $f \in 0$ (cf., for example, Kupershmidt[12]). Thus we have the lemma. Q.E.D.

4. The twisted multivariational operators

Let M be a vector space with k mutually commuting endomorphisms $\partial_1, \ldots, \partial_k$. Let

$$A_{M,k} := M \otimes A^{\otimes k},$$

where $A^{\otimes k} = A \otimes \cdots \otimes A$ (k times). Let

$$d_i = \partial_i \otimes 1 + 1 \otimes (1 \otimes \cdots \otimes 1 \otimes d \otimes 1 \otimes \cdots \otimes 1),$$

d being on the ith factor. Define

$$\delta_i := \sum (-d_i)^n \circ \frac{\partial}{\partial u_n},$$

$$\delta := \delta_1 \circ \cdots \circ \delta_n.$$

Then we have the following lemma.

Lemma B.4: Let P be a subspace of M invariant with respect to the d_i's. Then

$$\delta^{-1}(A_{P,k}) = \sum_{i=1}^{k} \operatorname{Im} d_i + M \otimes \mathsf{R}^{\otimes k} + A_{P,k}.$$

Proof: It is easy to see as before $\delta d_i = 0$ ($i = 1, \ldots, k$), whence δ maps the right-hand side into $A_{P,k}$.

Suppose $g \in A_{M,k}$ satisfies $\delta g \in A_{P,k}$. Then, mod Σ Im d_i,

$$\sum (\partial_{1,i_1} \cdots \partial_{k,i_k} g) \cdot u_{i_1} \otimes \cdots \otimes u_{i_k} \equiv \delta g \cdot u \otimes \cdots \otimes u \in A_{P,k},$$

where $\partial_{a,m} = 1 \otimes (1 \otimes \cdots \otimes 1 \otimes \partial/\partial u_m \otimes 1 \otimes \cdots \otimes 1)$, $\partial/\partial u_m$ being on the ath factor, and $A_{M,k}$ is considered as an $A^{\otimes k}$ algebra in the natural way. Now the argument in the proof of Lemma B.2 shows $g \in M \otimes \mathsf{R}^{\otimes k} + \Sigma \operatorname{Im} d_i + A_{P,k}$. Q.E.D.

For $K \in A$, define endomorphisms $X_{K,i}$, $D_{K,i}$ ($i = 1, \ldots, k$) of $A_{M,k}$ by

$$X_{K,i} := 1 \otimes (1 \otimes \cdots \otimes 1 \otimes X_K \otimes 1 \otimes \cdots \otimes 1),$$

$$D_{K,i} := \sum_{n=0}^{\infty} (-d_i)^n \circ \left(1 \otimes \cdots \otimes 1 \otimes \frac{\partial K}{\partial u_n} \otimes 1 \otimes \cdots \otimes 1 \right),$$

where X_K and $\partial K/\partial u_n$ are on the ith factor. Then we have the following lemma.

Lemma B.5: (i) If $i \neq j$, then δ_i commutes with $X_{K,j}$ and $D_{K,j}$. (ii) $\delta_i \circ X_{K,i} = (X_{K,i} + D_{K,i}) \circ \delta_i$. Q.E.D.

Proof: (i) is obvious and (ii) can be proved just in the same way as Lemma B.3. Q.E.D.

Corollary B.6: $\delta \circ X_{K,i} = (X_{K,i} + D_{K,i}) \circ \delta$.

Finally suppose $M = \mathsf{R}$, $\delta_i = 0$. Then Lemma B.4 implies the following lemma.

Lemma B.7: Let Q be a complement of $\mathsf{R} + \operatorname{Im} d$ in A. Then δ is injective on $Q^{\otimes k}$.

Proof: Obvious since $Q^{\otimes k}$ is a complement of Σ Im d_i in $A^{\otimes k}$. Q.E.D.

APPENDIX C: CONSERVATION LAWS OF THE KdV EQUATION

1. A complex associated to the KdV equation

Define a complex

$$0 \to \Omega^0 \xrightarrow{D} \Omega^1 \xrightarrow{D} \Omega^2 \to 0$$

as follows: Let

$$\Omega^i := A \otimes \wedge^i[dx, dt],$$

where $\wedge^*[dx, dt]$ stands for the exterior algebra on $\mathsf{R}\, dx \otimes \mathsf{R}\, dt$ and D is determined by

$$Df = df\, dx + d_t f\, dt, \quad \text{for } f \in A = \Omega^0,$$

$$D(g \wedge h) = Dg \wedge h + (-1)^a g \wedge Dh, \quad \text{for } g \in \Omega^a,\ h \in \Omega^b,$$

where $d_t = X_{uu_1 + u_3}$ in the notation of Appendix B 3. Since d and d_t commute with each other, we obtain a complex $\{\Omega^*, D\}$. Denote by H^i the ith cohomology space. We may call H^1 the space of the equivalence classes of conserved densities of the KdV equation, since Propositions 3.1, 3.2, and

4.3 for $k=1$ imply that the map $f\,dx+g\,dt\to\chi_1(1\otimes f)$ induces a map

$$H^1\to\operatorname{Ker} D_t\cap F^1\mathscr{P}(F(T))\,,$$

which in fact is an isomorphism by the argument before (5) in Sec. V.

Now we cite the result of Miura *et al.*[6] in the following form.

Theorem C.1: For each positive integer i, an element $w_i=I_i\,dx+X_i\,dt$ of Ω^1 exists such that $Dw_i=0$, weight$(w_i)=2i$. Moreover the classes in H^1 represented by the w_i's $(i=1,2,3,\ldots)$ are nonzero.

Let

$$\Delta:=D_K+X_K\quad\text{with } K=uu_1+u_3\,,$$

i.e.,

$$\Delta:=d_t-ud-d^3\,.$$

Then by Proposition B.2 and Lemma B.3, we have the following realization of H^1.

Lemma C.2: The map $I\,dx+X\,dt\to\delta_u I$ induces an injection $H^1\to\operatorname{Ker}\Delta$.

2. Computation of Ker Δ

Let

$$\Delta_{3,0}=\sum_{i,j,k=0}^{\infty}u_{i+1}u_{j+1}u_{k+1}\frac{\partial^3}{\partial u_i\partial u_j\partial u_k}+3\sum_{i,j=0}^{\infty}u_{i+2}u_{j+1}\frac{\partial^2}{\partial u_i\,\partial u_j}\,,$$

$$\Delta_{3,1}=-\sum_{i=0}^{\infty}\sum_{0<a\leqslant i}\binom{i}{a}\,u_a u_{i-a+1}\frac{\partial}{\partial u_i}\,.$$

Then it is easy to show the following lemma.

Lemma C.3:

(i) $\Delta=\Delta_{3,0}+\Delta_{3,1}$,

(ii) $\Delta_{3,1}(A^k(k))\subset A^{j+3}(k+i)$.

(iii) $\left[\frac{\partial}{\partial u},\Delta\right]=0$.

Now we solve the equation $\Delta f=0$.

Lemma C.4: Suppose $f\in A_n\setminus A_{n-1}$ satisfies $\Delta f=0$. Then n is even. Moreover, for $n\geqslant 4$,

$$f\equiv a(u_n+((n+1)/3)uu_{n-2})+bu_{n-1}+cu_{n-2}\pmod{A_{n-3}}\,,$$

and

$$f=a(u_2+u^2/2)+b\,,\quad\text{for } n=2\,,$$

$$f=a\,,\quad\text{for } n=0\,,$$

with $a,b,c\in\mathsf{R}$.

Proof: From $\partial/\partial u_{n+2}(\Delta f)=0$, we obtain

$$d\frac{\partial f}{\partial u_n}=0\,.$$

Hence by Lemma B.1, f must be of the form

$$f\equiv au_n\pmod{A_{n-1}}\,.$$

Thus for $n=0$ we obtain $f=au+b$. But then

$$\Delta f=au^2\,,$$

whence a must be zero.

Suppose now $n\geqslant 1$. Then

$$d\frac{\partial f}{\partial u_{n-1}}=\frac{\partial}{\partial u_{n+1}}\Delta f=0\,,$$

whence

$$f=au_n+bu_{n-1}+f_{n-2}\,,$$

with $a,b\in\mathsf{R}$ and $f_{n-2}\in A_{n-2}$.

Suppose $n=1$. Then $\Delta f=au_1^2+bu^2$, whence we have $a=0$, contradicting $f\notin A_0$.

Thus we have $n\geqslant 2$. Then from $(\partial/\partial u_{n-2})\Delta f=0$, we obtain

$$d\frac{\partial f_{n-2}}{\partial u_{n-2}}=\frac{(n+1)au_1}{3}\,,$$

whence

$$\frac{\partial f_{n-2}}{\partial u_{n-2}}=\frac{(n+1)au}{3}+c$$

with $a,c\in\mathsf{R}$.

Suppose now $n=2$. Then

$$f_0=u^2/2+cu+e$$

with an $e\in\mathsf{R}$, whence

$$f=a(u_2+u^2/2)+bu_1+cu+e\,.$$

But then $\Delta f=bu_1^2+cu^2$, whence $b=c=0$.

Suppose now $n\geqslant 3$. Then

$$f_{n-2}\equiv(n+1)auu_{n-2}/3+cu_{n-2}\pmod{A_{n-3}}\,.$$

Hence

$$f\equiv a(u_n+(n+1)uu_{n-2}/3)+bu_{n-1}+cu_{n-2}\pmod{A_{n-3}}\,.$$

Thus it remains to show that n is even. By (iii) of Lemma C.3, $\Delta\,\partial^k f/\partial u^k=0$ for any k. Hence if n is odd, we obtain an element of the form $au_1+g(u)$ in Ker Δ. Then by what we have shown above we must have $a=0$, contradicting $f\notin A_{n-1}$. Q.E.D.

Corollary C.5: Ker $\Delta\cap A_n^{n+3}=(0)$, for $n\geqslant 1$.

Proof: Suppose we have a nonzero element f in Ker $\Delta\cap A_n^{n+3}$. Note that $A_n^{n+3}=A_{n-1}^{n+3}$, since weight$(u_n)=n+2$, and weight$(u_j)\geqslant 2$ for all j. Thus $f\in A_k\setminus A_{k-1}$ for some k with $0\leqslant k\leqslant n-1$. By the above lemma, we have $f\equiv au_k\pmod{A_{k-1}}$. But weight$(u_k)=k+2\leqslant n+3$, whence $a=0$ contradicting $f\notin A_{k-1}$. Q.E.D.

Put $T_i=\delta_u I_i$, where the I_i's are those differential polynomials given in Theorem C.1. Then we have the following proposition.

Proposition C.6:

(i) Ker $\Delta\cap A^n=\begin{cases}\mathsf{R}\cdot T_{i+1}\,, & \text{for } n=2i\,,\\ (0)\,, & \text{for odd } n\,.\end{cases}$

(ii) $T_1=c_1\,,\quad T_2=c_2u\,,$

$$T_3=c_3(u_2+u^2/2)\,,$$

$$T_i=c_i(u_{2i-4}+(2i-3)uu_{2i-5}/3)\pmod{A_{2i-5}}$$

for $i\geqslant 4$ with nonzero c_i's.

Proof: Note first that $A^n = A^n_{n-2}$. Hence if n is odd, $\mathrm{Ker}\,\Delta \cap A^n = \mathrm{Ker}\,\Delta \cap A^n_{n-2} = \mathrm{Ker}\,\Delta \cap A^n_{n-3} = 0$ by Lemma C.4 and Corollary C.5.

Obviously we have $T_{i+1} \in A^{2i} = A^{2i}_{2i-2}$, which is non-zero. Suppose now $T \in \mathrm{Ker}\,\Delta \cap A^{2i} = \mathrm{Ker}\,\Delta \cap A^{2i}_{2i-2}$. Then by Lemma C.4

$$T \equiv a u_{2i-2} \pmod{A_{2i-3}},$$

whence $T - bT_{i+1} \in A^{2i}_{2i-3} \cap \mathrm{Ker}\,\Delta = (0)$ for some $b \in \mathsf{R}$. Hence $A^{2i} \cap \mathrm{Ker}\,\Delta = \mathsf{R}.T_{i+1}$, which gives (i).

Finally Lemma C.4 gives (ii). Q.E.D.

3. Information on certain differential polynomials

First we refine Theorem C.1 using Lemma C.2 and Proposition C.6.

Theorem C.7: For each positive integer i, an element $w_i = I_i\,dx + X_i\,dt$ of Ω^1 exists such that $Dw_i = 0$, $\mathrm{weight}(I_i) = 2i$, $\mathrm{weight}(X_i) = 2i+2$,

$$I_1 = u,$$

$$I_i \equiv u_{i-2}^2 \pmod{A[3]}, \quad \text{for } i \geqslant 2,$$

$$X_1 = u_2 + u^2/2,$$

$$X_i = 2u_{i-2}u_i - u_{i-1}^2 \pmod{A[3]}, \quad \text{for } i \geqslant 2.$$

Moreover the classes in H^1 represented by the w_i's $(i = 1,2,\ldots)$ constitute a basis of H^1.

Proof: Lemma C.2 and (i) of Proposition C.6 imply obviously the last assertion.

It is obvious that w_1 satisfies $Dw_1 = 0$ and $\delta_u I_1 = 1$ also spans $\mathsf{R}T_1$.

Let $i \geqslant 2$. Let I_i' be any element of A^{2i} such that $\delta_u I_i' = T_i$. As an element of A^{2i}, we can write

$$I_i' \equiv \sum a u_{2i-2} + \sum_{k=0}^{i-2} a_k u_k u_{2i-4-k} \pmod{A[3]}.$$

But mod $\mathrm{Im}\,d$, $u_{2i-2} \equiv 0$ and $u_k u_{2i-4-k} \equiv (-1)^k u_{i-2}^2$. Hence we may suppose $I_i' \equiv a_i u_{i-2}^2 \pmod{A[3]}$. But then $\delta_u I_i' \equiv 2a_i u_{2i-4} \pmod{A[2]}$. Hence we must have $a_i \neq 0$. Thus we can take $I_i = I_i'/a_i$.

Now mod $A[3]$

$$d_t u_{i-2}^2 \equiv 2u_{i-2}u_{i+1} = d\left[2u_{i-2}u_i - u_{i-1}^2\right].$$

Since $dA(m) \subset A(m)$ and $\mathrm{Ker}\,d = \mathsf{R}$, the $X_i \in A^{2i+2}$ with $dX_i = d_t I_i$ must be of the form

$$X_i = 2u_{i-2}u_i - u_{i-1}^2 \pmod{A[3]}.$$

Q.E.D.

Define $T_{ij} := \delta_u(S(i,j)) \in A^{2(i+j)}$, where we recall

$$S(i,j) = -I_i X_j + I_j X_i.$$

An easy calculation using the above theorem shows the following lemma.

Lemma C.8: (i) For i,j with $j > i \geqslant 2$,

$$T_{ij} \equiv c_{ij} u_{i-2}^2 u_{2j-2} \pmod{A[4]}$$

with $c_{ij} \neq 0$.

(ii) For $i \geqslant 2$,

$$T_{1i} \equiv c_i u u_{2i-2} \pmod{A[3]}$$

with $c_i \neq 0$.

Corollary C.9: T_k $(k = 1,2,\ldots)$ and T_{ij} $(1 \leqslant i < j)$ are linearly independent.

Proof: It suffices to show that T_{i+1} and $T_{k,i-k}$ $(1 \leqslant k < [i/2])$ are linearly independent, which is obvious by Proposition C.6 and Lemma C.8. Q.E.D.

4. Twisting of Δ

Let M be an R-vector space with an endomorphism ∂: $M \to M$. Define $A_M := M \otimes A$ and

$$\mathrm{weight}(m \otimes f) = i, \quad \mathrm{degr}(m \otimes f) = j,$$

for $m \in M$ and $f \in A^i(j)$. We denote $M \otimes A^i$, $M \otimes A(j)$, $M \otimes A_n$, $M \otimes A^i(j)$, etc., respectively, by A^i_M, $A_M(j)$, $A_{M,n}$, $A^i_M(j)$, etc. Define

$$d^M := \partial \otimes 1 + 1 \otimes d,$$

$$\Delta^M := 1 \otimes d_t - u d^M - (d^M)^3 : A_M \to A_M.$$

Then we can decompose Δ^M:

$$\Delta^M = \sum \Delta^M_{i,j},$$

where $\Delta^M_{i,j}(A^k_M(n)) \subset A^{k+i}_M(n+j)$. Then it is easy to show the following lemma.

Lemma C.10:

$$\Delta^M_{0,0} = \partial^3 \otimes 1, \quad \Delta^M_{1,0} = 3\partial^2 \otimes d,$$

$$\Delta^M_{2,0} = 3\partial \otimes d^2, \quad \Delta^M_{2,1} = \partial \otimes u,$$

$$\Delta^M_{3,0} = 1 \otimes \Delta_{3,0}, \quad \Delta^M_{3,1} = 1 \otimes \Delta_{3,1},$$

and

$$\Delta^M_{i,j} = 0, \quad \text{otherwise}.$$

Let

$$\Delta^M_2 := \Delta^M_{2,0} + \Delta^M_{2,1}, \quad \Delta^M_3 := \Delta^M_{3,0} + \Delta^M_{3,1} = 1 \otimes \Delta.$$

By Proposition C.6, we have the following lemma.

Lemma C.11:

$$\mathrm{Ker}\,\Delta^M_3 \cap A^n_M = \begin{cases} M \otimes \mathsf{R}.T_{i+1}, & \text{for } n = 2i, \\ (0), & \text{for odd } n. \end{cases}$$

5. Independence of T_i and T_{jk} mod Im Δ

Let M and ∂ be as above.

Proposition C.12: Suppose $f_j \in A^j_M$ $(j = 2i-2, 2i-3)$ satisfies

$$\Delta^M_3 f_{2i-2} = 0, \tag{C1}$$

$$\Delta^M_2 f_{2i-2} + \Delta^M_3 f_{2i-3} = a \otimes T_{i+1} + \sum_{1<k<[(i-1)/2]} a_k \otimes T_{k,i-k}. \tag{C2}$$

Then $a + 3a_1 = 0$. Furthermore if a or a_1 is zero, then all a_k's are zero and $\Delta^M f_{2i-2} = 0$.

We need the following lemma.

Lemma C.13: Let p_2: $A_M \to A_M(2)$ be the projection. Then

$$P_2 \circ \Delta^M_3 : A^{2i-3}_M(1) \otimes A^{2i-3}_M(2) \to A^{2i}_m(2)$$

is injective and $M \otimes \mathsf{R}.uu_{2i-4}$ is a complement of its image.

Proof: Since

$$p_2\Delta_3^M(m\otimes u_j u_{2i-7-j})$$
$$= 3m\otimes(u_{j+2}u_{2i-6-j}+u_{j+1}u_{2i-5-j}),$$

for $0\leqslant j\leqslant i-4$, we have

$$m\otimes u_j u_{2i-4-j}$$
$$\equiv(-1)^{i+j}m\otimes u_{i-2}^2 \quad [\mathrm{mod}\, p_2\Delta_3^M A_M^{2i-3}(2)],$$

for $1\leqslant j\leqslant i-3$. Further mod $p_2\Delta_3^M A_M^{2i-3}(2)$

$$\Delta_3^M(m\otimes u_{2i-5}) = -m\otimes\sum_{j=1}^{2i-5}\binom{2i-5}{j}u_j u_{2i-4-j}$$
$$\equiv -m\otimes\sum_{j=1}^{2i-5}\binom{2i-5}{j}(-1)^{i+j}u_{i-2}^2$$
$$= (-1)^i m\otimes u_{i-2}^2.$$

Hence $p_2\circ\Delta_3(A_M^{2i-3}(1)\oplus A_M^{2i-3}(2))$ is spanned by $\{m\otimes u_j u_{2i-4-j};\ m\in M,\ 1\leqslant j\leqslant i-2\}$. The injectivity of $p_2\circ\Delta_3$ can be easily proved. Q.E.D.

Proof of Proposition C.12: By Lemma C.11, (C1) implies $f_{2i-2}=m\otimes T_i$ with some $m\in M$. Then the $A_M^i(1)$ component of (C2) gives $a=3\,\partial m$. On the other hand, by virtue of the above lemma, we obtain comparing the coefficients of uu_{2i-4} in (C2)

$$(2i-2)\partial m=(2i-1)a/3+a_1,$$

whence $a+3a_1=0$.

Suppose now $a=a_1=0$. We may suppose $i\geqslant 5$. Since $\partial m=0$, we have $\Delta^M f_{2i-2}=\Delta_3^M f_{2i-2}=0$, by virtue of Lemma C.10. Thus we have

$$\Delta_3^M f_{2i-3}=\sum_{2\leqslant k\leqslant[(i-1)/2]}a_k\otimes T_{k,i-k}. \tag{C3}$$

Hence by Lemma C.8,

$$\Delta_3^M f_{2i-3}=0 \quad (\mathrm{mod}\, A[3]).$$

By Lemma C.13 above, we have

$$f_{2i-3}\in A[3].$$

Hence we can write

$$f_{2i-3}\equiv\sum_{j=0}^{2i-9}g_j u_j \quad (\mathrm{mod}\, A_M[4]),$$

where $g_j\in A_M(2)\cap A_{M,j}$. If $j\geqslant i-4$, then

$$\mathrm{weight}(u_a u_j^2)=6+2j+a\geqslant 2i-2,$$

whence g_j cannot have a nonzero term having u_j as a factor. Thus actually

$$g_j\in A_{M,j-1}, \quad \text{for } j\geqslant i-4.$$

Thus (C3) can be written as

$$\Delta_3^M(g_{2i-9}u_{2i-9}+\cdots+g_{i-4}u_{i-4}+h_{i-5})$$
$$\equiv\sum_{2\leqslant k\leqslant[(i-1)/2]}a_k\otimes T_{k,i-k}, \tag{C4}$$

mod $A_M[4]$ with $g_j\in A_{M,j-1}$ and $h_{i-5}\in A_{M,i-5}$.

Consider now the following assertion:

$$\begin{cases} a_j=0, & \text{for } j\leqslant k,\\ g_j=0, & \text{for } j\geqslant 2i-2k-4. \end{cases} \tag{C5}_k$$

What we must show is $(C5)_{p-1}$ when $i=2p$ and $(C5)_p$ when $i=2p+1$. In either case we have only to show $(C5)_{[(i-1)/2]}$, which we shall prove by induction on k.

First, comparing the coefficients of u^2u_{2i-6} of (C4), we have $a_2=0$. Hence $(C5)_2$ is valid if we consider g_j to be zero for $j\geqslant 2i-8$.

Suppose now that for some k such that $2\leqslant k\leqslant[(i-1)/2]-1$ the assertion $(C5)_k$ is true. Then (C4) looks like

$$\Delta_3^M(g_{2i-2k-5}u_{2i-2k-5}+g_{2i-2k-6}u_{2i-2k-6}+\cdots)$$
$$\equiv a_{k+1}\otimes(u_{k-1}^2u_{2i-2k-4}+\cdots)+\cdots \tag{C6}$$

mod $A_M[4]$. Since $k\leqslant[(i-1)/2-1]$, we have $2i-2k-6\geqslant i-4$, whence

$$g_s\in A_{M,s-1} \quad \text{for } s=2i-2k-5,\ 2i-2k-6.$$

Comparing the coefficients of $u_{2i-2k-3}$ in (C6), we obtain

$$(1\otimes d)f_{2i-2k-5}=0.$$

This implies by Lemma B.1, $g_{2i-2k-5}=0$. Comparing further the coefficients of $u_{2i-2k-4}$ in (C6), we obtain

$$(1\otimes d)g_{2i-2k-6}=a_{k+1}\otimes u_{k-1}^2.$$

Applying $1\otimes\delta_u$, we obtain $a_{k+1}\otimes u_{2k-2}=0$, whence $a_{k+1}=0$. Then we have $g_{2i-2k-6}=0$, establishing $(C5)_{k+1}$. Q.E.D.

6. A refinement of Proposition C.6

Let M and ∂ be as in Appendix C 4 and G an endomorphism of M.

Lemma C.14: $\mathrm{Ker}(\Delta^M+G\otimes 1)=(\mathrm{Ker}\,G\cap\mathrm{Ker}\,\partial)\otimes\tilde{T}$, where $\tilde{T}$ is the subspace of A spanned by T_i's.

Proof: Suppose $g\in A_M$ satisfies

$$(\Delta^M+G\otimes 1)g=0. \tag{C7}$$

Let g_k be the A_M^k component of g and n the maximal number such that $g_n\neq 0$. The A_M^{n+3} component of (C7) gives $\Delta_3^M g_n=0$, whence by Lemma C.11, n is even: $n=2i$ and $g_{2i}=a_1\otimes T_{i+1}$ for some $a_1\in M$. Then the A_M^{2i+2} component of (C7) gives

$$\partial a_1\otimes(3d^2T_{i+1}+uT_{i+1})+\Delta_3^M g_{2i-1}=0.$$

Since $\mathrm{Im}\,\Delta_3^M\cap A_M(1)=0$, we obtain $\partial a_1=0$ if we compare the coefficients of u_{2i}. Thus we have $\Delta^M(a_1\otimes T_{i+1})=0$ and $\Delta_3^M g_{2i-1}=0$, whence $g_{2i-1}=0$.

Now the A_M^{2i+1} component of (C7) reads $\Delta_3^M g_{2i-2}=0$, whence $g_{2i-2}=a_2\otimes T_i$ for some $a_2\in M$.

Finally the A_M^{2i} component of (C7) gives

$$G(a_1)\otimes T_{i+1}+\partial a_2\otimes(3d^2T_i+uT_i)+\Delta_3^M g_{2i-3}=0. \tag{C8}$$

By Lemma C.13, the coefficients of u_{2i-2} and uu_{2i-4} in (C8) give when $i\geqslant 3$

$$G(a_1)+3\,\partial a_2=0,$$
$$(2i-1)G(a_1)/3+(2i-2)\partial a_2=0, \tag{C9}$$

whence $G(a_1)=0$. When $i=2$, (C9) is replaced by

$$G(a_1)+\partial a_2=0,$$

whence $G(a_1)=0$ again. Finally when $i=1$, we have

$$g=a_1\otimes u+a_2\otimes 1,$$
$$(\Delta^M+G\otimes 1)g=G(a_1)\otimes u+G(a_2)\otimes 1=0,$$

whence $G(a_1) = 0$.

Thus we have

$$a_1 \otimes T_{i+1} \in (\mathrm{Ker}\, G \cap \mathrm{Ker}\, \partial) \otimes \tilde{T}$$

and

$$g - a_1 \otimes T_{i+1} \in A_M^{n-1}.$$

Hence by the induction on n, we obtain the Lemma. Q.E.D.

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Minimization of Landau potentials invariant under SO(3)

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The absolute minima for Landau potentials corresponding to one irreducible representation of SO(3) of spin up to 4 are computed together with their stability groups. For spin 4 the nonmaximal D_4 stability group appears. This is a contribution to the literature about Michel's conjecture.

I. INTRODUCTION

The relevance of the concept of spontaneous symmetry breaking in physics is so well known that there is no point in commenting on it at length. Indeed, it enters crucially in the description of well understood phenomena like, for example, superconductivity or ferromagnetism. It also plays an essential role in the theory of electroweak interaction within the Higgs sector of the standard model.

The success of these models encouraged physicists to look for theories describing other interactions by means of a unique gauge group unbroken at high energy but spontaneously broken at current energy in order to describe the observed world. Until now, it is always a scalar field (Landau field) that realizes the breakdown by acquiring a nonvanishing expectation value through the minimization of a suitably chosen self-interacting potential (Landau potential).

The breakdown patterns raise the following problem. Given a group G, a field Ψ transforming according to a representation of G (reducible or irreducible) and a polynomial $V(\Psi)$ (of degree less than or equal to 4) invariant under the action of the group, find the configurations Ψ that realize the absolute minimum of V.

Following the point of view of model builders, it is the unbroken group (the little group or stability group of Ψ) that is important for physics; indeed this subgroup of G has to contain all the symmetries observed at the current energy in order for the model to be acceptable.

The problem of finding the extreme Ψ's and their corresponding stability groups becomes rapidly untractable when one chooses for Ψ representations of high dimensions of the most popular groups as required in many great unification models.

As an attempt to know *a priori* which breaking patterns are possible, Michel's conjecture,[1,2] in its simplest form, states that the only possible stability groups for irreducible Ψ's are maximal subgroups of the group G.

After it was proposed, this conjecture provided an interesting and exciting challenge for the theoreticians: to prove it completely or to disprove it by constructing some counterexamples.

The conjecture was first verified explicitly for up to two index tensors which are irreducible representations of SU(N) and SO(N).[3,4] Unfortunately some years ago, a first counterexample was discovered in the framework of SU(5) with the 75-dimensional representation.[5] Later on, other counterexamples were constructed based on the 27-dimensional representation of SU(3).[6]

Afterwards, a big activity was developed around these works in order to try to bypass the conjecture or to improve it.[7–9]

In order to contribute to the study of the problem, we have decided to compute as explicitly as possible the minimization of Landau potentials invariant under the simplest of all simple Lie groups: SO(3). We obtain detailed answers for irreducible representations of spin up to four ($s = 1,2,3,4$).

We show in particular the importance played by finite subgroups of SO(3) as stability groups of the Landau potential, and obtain counterexamples to Michel's conjecture.

Section II contains generalities concerning the problem and fixes the notations. It also exhibits a table summarizing the number of invariants and the possible stability groups for the irreducible representation considered. In Sec. III the explicit results for spin 1, 2, 3, and 4 are presented. In particular it is shown that the conjecture always holds for $s = 1$, 2, and 3. For $s = 4$ and for suitable choices of the parameters of the Landau potential some minima are invariant under D_4, a nonmaximal finite subgroup of SO(3).

In Sec. IV we present our conclusions and recall some of our technical contributions.

II. GENERALITIES. NOTATIONS

A. Irreducible representations. Invariants. Landau potential

Irreducible representations of the Lie group SO(3) have integer spin s and are completely characterized by their dimension $d = 2s + 1$. The space on which the representation acts may be described by completely symmetric, traceless tensors S with s indices a ranging from 1 to 3; i.e.,

$$S_{a_1 a_2 \cdots a_s} = S_{a_{i_1} a_{i_2} \cdots a_{i_s}}, \tag{2.1}$$

where $i_1, i_2, \ldots, i_s$ is an arbitrary permutation of $1,2,\ldots,s$ and

$$\sum_{a=1}^{3} S_{aaa_3 \cdots a_s} = 0. \tag{2.2}$$

Given s, group invariants can be constructed by saturation of indices among products of several S's. The simplest example is the norm of S (say Q),

$$Q = S_{a_1 a_2 \cdots a_s} S_{a_1 a_2 \cdots a_s}, \tag{2.3}$$

where the summation on the dummy indices is understood.

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For $s>1$, however, there exist other independent invariants with degree higher than 2 (see Table I).

A Landau potential is a group invariant polynomial in the variable S. Being a part of an action density of a field theory, the degree of this polynomial is required to be less than or equal to 4 for renormalizability.

Let P_m $(m=1,...,M)$ be all the independent invariants cubic in S and let Q^2, K_n $(n=1,...,N)$ be all the independent invariants quartic in S. Denote also

$$\{I_k\}=\{Q,P_m,K_n\},\quad k=1,...,M+N+1, \tag{2.4}$$

the set of all independent invariants of degree lower than or equal to 4. The numbers M and N are given in Table I for s up to 7. It is to be remarked that M equals zero for s odd and one for s even.

The most general renormalizable Landau potential

$$V=2\mu Q+qQ^2+\sum_{m=1}^{M}p_mP_m+\sum_{n=1}^{N}k_nK_n \tag{2.5}$$

depends on $2+M+N$ independent coupling constants (μ, q, the p's and the k's).

A necessary condition for it to be physically acceptable is that it increases when S goes to infinity in any direction: this is the asymptotic positivity condition which implies some relations between q and the k's which are supposed not to be all zero (see Sec. II E).

Let us finally remark that (2.5) is by construction SO(3) invariant. However, in certain cases when the coupling constants take specific values, the potentials may be invariant under a larger group. These accidental symmetries may often be difficult to find but should in principle not be ignored.

For example, for s odd or for s even when the p's are zero, V has a parity ($S\to -S$) as accidental symmetry. The potential is then invariant under O(3) rather than SO(3). Except for casual remarks this fact will not be insisted upon later. Note also that when all the p's and all the k's are zero, the potential is invariant under the much larger accidental group $O(2s+1)$.

TABLE I. The number of independent invariants cubic in S (M), quartic in S (N) (excluding Q squared), and the total number of invariants including the quadratic one Q ($1+M+N$) are presented for values of s up to 7. The list of all possible stability groups, as subgroups of SO(3), compatible with the representation labeled by s, is also given. See Appendix A for notations. When s is odd the extension by parity can be trivially made. We note the absence of the stability group D_2 in the case of $s=3$ in contrast with Table A.11 of Ref. 10. In fact we have remarked that in this case invariance under D_2 automatically implies invariance under T (the group of the tetrahedron).

s	M	N	$1+M+N$	Possible stability groups
1	0	0	1	C_∞,SO(3)
2	1	0	2	D_2,D_∞,SO(3)
3	0	1	2	E,C_2,C_3,D_3,T,C_∞,SO(3)
4	1	1	3	$E,C_2,D_2,D_3,D_4,O,D_\infty$,SO(3)
5	0	1	2	$E,C_{2,...,5},D_{2,...,5},C_\infty$,SO(3)
6	1	2	4	$E,C_{2,3},D_{2,...,6},T,O,Y,D_\infty$,SO(3)
7	0	3	4	$E,C_{2,...,7},D_{2,...,7},T,C_\infty$,SO(3)

B. Maximality equations, orbits, strata, and stability groups

Given one Landau potential (2.5) for one irreducible representation of SO(3) of dimension d the equations for the extrema of V are the d equations

$$\partial V=\frac{\partial V}{\partial S}=\sum_{k=1}^{1+M+N}\frac{\partial V}{\partial I_k}\frac{\partial I_k}{\partial S}=0$$

$$=\sum_{k=1}^{1+M+N}\frac{\partial V}{\partial I_k}\partial I_k. \tag{2.6}$$

In general these equations imply that the $(1+M+N)$ d-dimensional vectors ∂I be linearly dependent. They lead to systems of cubic equations in the components of S.

A solution of (2.6) will be a local minimal of V provided that the $d\times d$ symmetric Hessian tensor

$$H=\frac{\partial^2 V}{\partial S\,\partial S} \tag{2.7}$$

has no negative eigenvalue.

Given one solution of (2.6) other solutions can be found by performing an arbitrary rotation on it, generating the orbit of the solution.

An essential property of a solution is its stability group, i.e., the subgroup of the invariance group of the potential that leaves S invariant. More restrictively we will be interested in the subgroup of SO(3) that leaves S invariant: i.e., the set of R such that

$$S_{a_1\cdots a_s}=R_{a_1b_1}\cdots R_{a_sb_s}S_{b_1\cdots b_s}. \tag{2.8}$$

All points on the same orbit have isomorphic stability groups. The union of all the orbits with isomorphic stability groups is called a stratum.

We now elaborate on this problem.

C. Stability groups as subgroups of SO(3)

The problem of finding the stability groups of a given configuration is difficult and interesting by itself. Fortunately in SO(3) it can be simplified due to the fact that any nontrivial rotation has one and only one (normalized) eigenvector (say x) with eigenvalue unity,

$$R_{ab}x_b=x_a, \tag{2.9}$$

corresponding to the axis of the rotation.

Now, contracting Eq. (2.8) $s-1$ times with x gives the following relation:

$$R_{ba}y_a=y_b, \tag{2.10}$$

where, by definition,

$$y_a=S_{aa_2a_3\cdots a_s}x_{a_2}x_{a_3}\cdots x_{a_s}. \tag{2.11}$$

As a consequence the vectors y and x have to be proportional and

$$S_{aa_2\cdots a_s}x_{a_2}\cdots x_{a_s}=\lambda x_a \tag{2.12}$$

providing a generalized (nonlinear) eigenvalue equation for the axes of rotations of the stability group of S. It should be stressed that Eq. (2.12) is a necessary condition; not all of its solutions are axes but the knowledge of the solutions x and their scalar products simplifies the search of the stability group.

In Table I, for s up to 7, we list all the possible stability groups compatible with the representation labeled by s. (See Appendix A for notation.)

Let us notice the absence of stability group D_2 in the case $s=3$ in contrast with Table A.11 of Ref. 10. In fact, we have remarked that in this case invariance under this group automatically implies invariance under T (the group of the tetrahedron).

D. Line of attack

In order to attack Eq. (2.6) two different routes have retained our attention. The first one consists in solving the equations by combination and factorization. Then one computes the stability group of any solution by using Eq. (2.12). This method has been applied successfully for the cases $s \leqslant 3$. In the case $s=4$, it leads to heavy computations that we did not manage to perform completely.

For this reason, we developed a second approach, more intimately related to the classification of Table I. For each stability group compatible with $s=4$, we construct a configuration of S invariant under this group and solve the new systems obtained by substitution of our ansatz in Eq. (2.6). The different invariants and the explicit values of the potential can then be computed for any of these configurations. Numerical plots of these values in terms of the coupling constants determine in which configuration the absolute minimum is attained. Finally the results have been tested by computer by minimizing the potential for randomly chosen values of the coupling constants and comparing the numerical minimum with the values obtained analytically by our method.

E. Asymptotic positivity condition

In order to be physically relevant, the Landau potential has to be bounded from below. This statement is equivalent to the requirement that the quartic part of V [say $V(4)$] be a positive definite homogeneous function. So, we have to impose positivity on any ellipsoidal-type hypersurface around the origin in the configuration space; a particularly convenient surface to use is $Q=1$.

Moreover, due to the compactness of such a surface, it is sufficient to check positivity in the extremal direction of the function

$$W = V(4) + \lambda(Q-1), \tag{2.13}$$

where the constraint has been implemented by use of a Lagrange parameter. Extrema of the function W obey

$$\partial W = \partial V(4) + \lambda\, \partial Q. \tag{2.14}$$

This equation is of the same form as (2.6) since W is analogous to V for other values of the coupling constants.

In conclusion, we stress that one has to impose positivity of the quartic part of V only on the directions corresponding to extrema of W in order to fulfill the asymptotic positivity condition.

F. Canonical position

Since V is invariant under the group SO(3), which transforms solutions of the maximality equation (2.6) into solutions, it is possible, using rotations, to fix up three parameters of the tensor S. In other words S can be put in a canonical position. In the example of the next section, we will use this freedom to simplify calculations. However, for $s>2$ this operation is not as straightforward as in the case of $s=1$ where S, a vector, can be put in the z direction or in the $s=2$ case where S, a symmetric matrix, can be diagonalized.

In order to define a canonical position in the general case we have found convenient to define it as follows. Let $\tilde{S}$ be a particularly simple fixed tensor S. When a generic tensor S' is allowed to rotate under SO(3) according to (2.8) or more compactly

$$S = RS', \tag{2.15}$$

its scalar product with $\tilde{S}$

$$F = (\tilde{S},S) = \tilde{S}_{a_1a_2\cdots a_s} S_{a_1a_2\cdots a_s} \tag{2.16}$$

varies. The canonical S is then defined as that S for which the scalar product (2.16) is (locally) minimal. Around that S the equations are

$$\left.\frac{\partial F}{\partial R}\right|_{R=1} = 0, \tag{2.17}$$

where the derivatives can be taken with respect to the parameters of the infinitesimal rotations R. In general (2.17) implies three linear relations among the components of S, providing the canonization associated with the ansatz $\tilde{S}$.

It is understood that all differentials in Eqs. (2.6), (2.7), and (2.14) are taken with respect to the full variations around a canonical position. Canonization is implemented on the vectors ∂Q, ∂I, etc., after the derivations have been performed. In other words, ∂I are $(2s+1)$-dimensional vectors depending on $2s-2$ parameters only. This reduction simplifies the computations considerably.

III. DISCUSSION OF THE MAXIMAL SOLUTIONS FOR s UP TO 4

In this section, using the notations and the general ideas presented in the preceding section, we present a discussion of the maximal solutions for s up to 4.

A. The $s=1$ case

This case is completely obvious but let us recall it for completeness. The only invariant is Q, the length squared of the vector S, and

$$V = 2\mu Q + qQ^2. \tag{3.1}$$

Choosing $\tilde{S}$ to be the z axis (0,0,1) the canonical position is (0,0,c) as can be verified easily. Maximalization of (3.1) leads to

$$\partial V = 2(\mu + qQ)\partial Q = 0. \tag{3.2}$$

Apart from the trivial solution $S=0$ [which is always present and has SO(3) as the stability group], Eq. (3.2) simply fixes the length (squared) of S in terms of μ and q,

$$Q = -\mu/q, \tag{3.3}$$

and the potential becomes

$$V = -\mu^2/q. \tag{3.4}$$

This implies that μ is negative since q must be positive by the

asymptotic positivity condition. This case is the celebrated example of spontaneous symmetry breaking of SO(3). The stability group of its solution is SO(2) [better O(2) if the accidental symmetry of parity is taken into account], i.e., a maximal subgroup of SO(3) [better O(3)] in this representation.

B. The $s=2$ case

This case is also well known. There are two independent invariants, associated with the 3×3 symmetric traceless matrix S,

$$Q = \mathrm{Tr}\, S^2, \tag{3.5}$$

$$P = \mathrm{Tr}\, S^3. \tag{3.6}$$

The Landau potential can then be chosen as

$$V = 2\mu Q + pP + qQ^2, \tag{3.7}$$

where the asymptotic positivity condition requires q to be positive. If $\tilde{S}$ in (2.16) is chosen to be diagonal with all three elements different from each other, the canonical position of S is diagonal in agreement with the allowed diagonalization of a symmetric matrix

$$S = \mathrm{diag}(\alpha,\beta,\gamma), \quad \alpha+\beta+\gamma = 0. \tag{3.8}$$

The equation for the minima (2.6) is

$$\partial V = 2(\mu + qQ)\partial Q + p\,\partial P = 0 \tag{3.9}$$

and it is easy to see that the two five-vectors ∂Q and ∂P are proportional only if two of the eigenvalues in Eq. (3.8) (say $\beta=\alpha, \gamma=-2\alpha$) are equal. As a consequence the stability group of the minimum is a SO(2) subgroup of SO(3), i.e., a maximal subgroup compatible with the $s=2$ representation of SO(3).

The extrema of V are then obtained for

$$\alpha = (3p + \epsilon\Delta)/48q, \tag{3.10}$$

where ϵ is an arbitrary sign and Δ is the positive square root of

$$\Delta^2 = 3(3p^2 - 128\mu q). \tag{3.11}$$

This implies

$$3p^2 > 128\mu q. \tag{3.12}$$

The value for the lowest extreme V is

$$V_{\mathrm{ext}} = -(2^{11}3^2q^3)^{-1} \times (3^3p^4 + p\Delta^3 - 2^6 3^3 \mu q p^2 + 2^{11}3^2\mu^2 q^2), \tag{3.13}$$

where Δ is the positive square root of (3.11). The negative square root corresponds to a higher potential.

Formulas (3.10) and (3.13) obviously fail when q goes to zero. However, the asymptotic positivity condition implies that q be strictly positive. Hence there is no problem.

The case p equal to zero is peculiar. Indeed, as explained in Sec. II A, the accidental invariance is O(5) and (3.3) and (3.4) hold.

C. $s=3$ case

In this case, three invariants can be constructed out of S:

$$Q = S_{abc}S_{abc}, \tag{3.14a}$$

$$K = S_{abf}S_{abg}S_{cdf}S_{cdg}, \tag{3.14b}$$

$$K' = S_{abc}S_{ade}S_{bdf}S_{cef}, \tag{3.14c}$$

they are not independent since they are related through the nonlinear identity

$$Q^2 - 2K - 2K' = 0. \tag{3.15}$$

Therefore, we can eliminate K' in favor of K and consider the Landau potential given by

$$V = 2\mu Q + qQ^2 + kK. \tag{3.16}$$

Quite generally the seven independent components of S can be written

$$\begin{aligned} &S_{122}=A, \quad S_{133}=A', \quad S_{111}=-A-A', \\ &S_{233}=B, \quad S_{112}=B', \quad S_{222}=-B-B', \\ &S_{113}=C, \quad S_{223}=C', \quad S_{333}=-C-C', \\ &S_{123}=S. \end{aligned} \tag{3.17}$$

The invariance of V can be exploited, in the manner described in Sec. II F, to put S into a canonical position and hence fix three relations between its components. Taking $\tilde{S}$ such that [see (2.16) and (2.17)]

$$\tilde{S}_{123} = 1, \quad \tilde{S}_{aab} = 0 \text{ (no sum over } a), \tag{3.18}$$

the canonical position associated with this ansatz can be summarized as (3.17) with the restrictions

$$A = A', \quad B = B', \quad C = C'. \tag{3.19}$$

In terms of the restricted parameters A, B, C, S the invariants (3.14) take the form

$$Q = 10(A^2+B^2+C^2) + 6S^2, \tag{3.20}$$

$$\begin{aligned} K = {} & 44(A^4+B^4+C^4) + 12S^4 \\ & + 50(A^2B^2 + A^2C^2 + B^2C^2) \\ & + 64S^2(A^2+B^2+C^2) + 8((AB-CS)^2 \\ & + (AC-BS)^2 + (BC-AS)^2), \end{aligned} \tag{3.21}$$

and the conditions (2.6) become

$$\partial V = 2(\mu + qQ)\partial Q + k\,\partial K, \tag{3.22}$$

where ∂V,... denoted differentials with respect to the whole seven-parameter phase space; relations (3.19) can be imposed only after the derivation has been carried out.

We again discard the $k=0$ solutions whose discussion is identical to the $s=2$ corresponding case [higher accidental symmetry, here O(7)].

More interesting solutions are available when k is different from zero; in particular, (3.22) implies that the seven-vectors ∂Q and ∂K be proportionnal. Table II summarizes the values of the parameters of the different configuration solutions of the equations for μ negative. For each case, the stability group is also presented. For μ positive, S and V are zero.

The knowledge of Table II allows to compute the invariants and the potential V [see (3.16)] as a function of μ, q, and k. This information is given in Table III. It is to be remarked that in all cases the value of the quadratic part of V is equal to twice V,

$$2\mu Q = +2V, \tag{3.23}$$

while the quartic part is equal to minus V,

$$qQ^2 + kK = -V. \tag{3.24}$$

TABLE II. Solutions for the extreme configurations in canonical positions in the case $s = 3$. It is to be remarked that solutions 1 and 4a (and also 2 and 4b, 3 and 4c) are related through a rotation, i.e., that the corresponding S' are on the same orbit. Obviously also other solutions can be generated from 3 by exchanging A or B with C. In case 4 the signs of B and C can be changed provided S is changed by the product of both signs.

Case	A	B	C	S	Stability group	Value of the parameters
1	0	0	C	$\pm C$	D_3	$C^2 = -\mu/8(k+2q)$
2	0	0	0	S	T	$S^2 = -\mu/2(k+3q)$
3	0	0	C	0	SO(2)	$C^2 = -5\mu/2(11k+25q)$
4a	A	A	A	$-2A$	D_3	$A^2 = -\mu/27(k+2q)$
4b	A	A	A	$A/4$	T	$A^2 = -8\mu/81(k+3q)$
4c	A	A	A	$5A/2$	SO(2)	$A^2 = -10\mu/27(11k+25q)$

As we know, the asymptotic positivity conditions are fulfilled when all maximal cases of the quartic part are positive. This implies (see Table II)

$$q + k/2 > 0, \tag{3.25a}$$

$$q + k/3 > 0, \tag{3.25b}$$

$$q + \tfrac{11}{25}k > 0. \tag{3.25c}$$

When k is positive, the effective condition is (3.25b), when k is negative it is (3.25a).

In the last two columns of Table III we give the absolute minima reached, respectively, by solutions 1 and 2 for k negative and k positive. The corresponding stability groups (respectively, T and D_3) are both maximal subgroups of SO(3) in the present representation. Notice, however, that the minima never occurs for case 3 despite the fact that the corresponding stability group SO(2) is a maximal subgroup of SO(3).

D. $s=4$ case

There are *a priori* five invariants of degree lower than 4 constructed out of S; a quadratic invariant

$$Q = S_{abcd}S_{abcd}, \tag{3.26a}$$

a cubic invariant

$$P = S_{abcd}S_{cdfg}S_{fgab}, \tag{3.26b}$$

and three quartic invariants

$$K = S_{abij}S_{abkl}S_{cdik}S_{cdjl}, \tag{3.26c}$$

TABLE III. The values of Q, K, and V are given for the nonequivalent cases of Table II for $s = 3$. In the last two columns the absolute minimum is given. For k positive, it corresponds to case 2 and stability group T. For k negative the minimum corresponds to case 1 and the stability group is D_3.

Case	Stability group	Q	K	V	$k<0$	$k>0$
1	D_3	$16C^2$	$128C^4$	$-\dfrac{\mu^2}{q+k/2}$	$q > -\dfrac{k}{2}$	
2	T	$6S^2$	$12S^4$	$-\dfrac{\mu^2}{q+k/3}$		$q > -\dfrac{k}{3}$
3	SO(2)	$10C^2$	$44C^4$	$-\dfrac{\mu^2}{q+11k/25}$		

$$K_1 = S_{abci}S_{abcj}S_{defi}S_{defj}, \tag{3.26d}$$

$$K_2 = S_{abcd}S_{cdef}S_{efgh}S_{ghab}. \tag{3.26e}$$

However, K_1 and K_2 can be eliminated in favor of K and Q thanks to the following nonlinear relations:

$$K_1 = \tfrac{1}{2}(Q^2 - 5K), \tag{3.27a}$$

$$K_2 = \tfrac{1}{2}(Q^2 - 8K). \tag{3.27b}$$

As a consequence the general Landau potential takes the form

$$V = 2\mu Q + pP + qQ^2 + kK \tag{3.28a}$$

with

$$p \geqslant 0. \tag{3.28b}$$

Indeed V is invariant under the symmetry that changes the signs of S and p. Hence p can be chosen to be non-negative by suitably adjusting the sign of S.

Quite generally S depends on nine parameters

$$\begin{aligned} &S_{2223} = A, \quad S_{2333} = A', \quad S_{1333} = B, \\ &S_{1113} = B', \quad S_{1112} = C, \quad S_{1222} = C', \\ &S_{2233} = \alpha, \quad S_{1133} = \beta, \quad S_{1122} = \gamma, \end{aligned} \tag{3.29}$$

with S completely symmetrical and by the trace conditions

$$\begin{aligned} &S_{1111} = -\beta - \gamma, \quad S_{2222} = -\alpha - \gamma, \\ &S_{3333} = -\alpha - \beta, \quad S_{1123} = -A - A', \\ &S_{1223} = -B - B', \quad S_{1233} = -C - C'. \end{aligned} \tag{3.30}$$

With the choice

$$\begin{aligned} &\tilde{S}_{1111} = \tilde{S}_{2222} = \tilde{S}_{3333} = -2, \\ &\tilde{S}_{1122} = \tilde{S}_{2233} = \tilde{S}_{1133} = 1, \end{aligned} \tag{3.31}$$

for $\tilde{S}$ [see (2.16)], all the other $\tilde{S}$'s, with different indices, being zero, we find the canonical position of S in terms of six remaining parameters since (2.17) then implies

$$A = A', \quad B = B', \quad C = C'. \tag{3.32}$$

The invariants Q, P, and K can be expressed as (relatively) simple functions of the canonical parameters,

$$\begin{aligned} Q = 2(&28(A^2 + B^2 + C^2) + 4(\alpha^2 + \beta^2 + \gamma^2) \\ &+ (\alpha\beta + \beta\gamma + \gamma\alpha)), \end{aligned} \tag{3.33}$$

$$\begin{aligned} P = 6(&8ABC + 7(\alpha + \beta + \gamma)(A^2 + B^2 + C^2) \\ &+ 5(A^2\alpha + B^2\beta + C^2\gamma) + (\alpha^3 + \beta^3 + \gamma^3) \\ &- (\alpha^2 + \beta^2 + \gamma^2)(\alpha + \beta + \gamma) + \alpha\beta\gamma), \end{aligned} \tag{3.34}$$

$$\begin{aligned} K = 4(&48(A^4 + B^4 + C^4) + 75(A^2B^2 + A^2C^2 + C^2A^2) \\ &+ 52ABC(\alpha + \beta + \gamma) \\ &+ 16(\alpha + \beta + \gamma)(A^2\alpha + B^2\beta + C^2\gamma) \\ &+ 3(A^2 + B^2 + C^2)(\alpha^2 + \beta^2 + \gamma^2) \\ &- 3(A^2\alpha^2 + B^2\beta^2 + C^2\gamma^2) \\ &- 18(A^2\beta\gamma + B^2\gamma\alpha + C^2\alpha\beta) \\ &+ 3(\alpha^2\beta^2 + \beta^2\gamma^2 + \gamma^2\alpha^2) + 2\alpha\beta\gamma(\alpha + \beta + \gamma)). \end{aligned} \tag{3.35}$$

The function K is positive (this was checked by computer) but not positive definite as a configuration like

$$A = B = C = \alpha = \beta = 0, \quad \gamma \neq 0 \tag{3.36}$$

annihilates K. As an obvious consequence the asymptotic positivity condition implies that q be strictly positive.

The extremal conditions associated with the potential (3.28)

$$\partial V = 2(\mu + qQ)\partial Q + p\,\partial P + k\,\partial K = 0, \tag{3.37}$$

imply that the three nine-dimensional vectors be linearly dependent.

Let D be the three by nine matrix

$$D = (\partial Q, \partial P, \partial K). \tag{3.38}$$

All 3×3 subdeterminants of D, which are homogeneous polynomials of degree 6 in the canonical parameters, have to vanish simultaneously in order for (3.37) to hold.

We have not succeeded in solving completely this system of nonlinear equations.

Instead we have chosen to analyze the problem by following another path based on a systematic exploration of the possible invariance groups compatible with the representation $s = 4$ under consideration (see Table I).

Since we now start with given stability groups we have to choose the axes of these groups in special position and compute the relative values of the components of the invariant S's.

Obviously a special stability group does not automatically lead to a canonical S [as defined in (3.32)]. But by a suitable transformation a special stability group can always be rotated in such a way that its related S becomes canonical.

In Table IV a certain number of useful special stability groups are defined and the corresponding S's (canonical or noncanonical) are given. They have been chosen to our best convenience. It is also clear that using suitable rotations any of these particular S's can be rotated to obtain stability groups of arbitrary orientation with respect to the special ones we have chosen.

In order to stress the subgroup embeddings, it should be remarked that certain subgroups have been given more than once with different directions of their symmetry axis. This allows one to write the two chain subgroup embeddings

$$\left.\begin{array}{l} C_2(z)\to D_2(z)\to D_4(z) \\ C_2(x)\to D_3(z) \end{array}\right\}\to D_\infty(z)\to \mathrm{SO}(3), \tag{3.39}$$

$$\left.\begin{array}{l} C_2(z)\to D_2(z)\to D_4(z) \\ C_2(m)\to D_3(d) \end{array}\right\}\to \mathrm{O}\to \mathrm{SO}(3), \tag{3.40}$$

which culminate in the two maximal embeddings D_∞ and the cube group O with special but particularly simple orientation.

Before analyzing the maximality equations (3.37) in each case let us give the asymptotic positivity conditions which read

$$k + 15q > 0, \quad q > 0. \tag{3.41}$$

Inserting any of the configurations of Table IV into Eq. (3.37) leads to restrictions for the remaining free S parameters depending on the potential coupling constants μ, p, q, and k. In fact, in general S can be computed in terms of the coupling constants. The invariants (3.26) and the potential (3.28) itself can then be evaluated.

Since these computations require quite a lot of algebra we have chosen to present the results only for the special stability groups of Table IV.

TABLE IV. The stability groups are defined in Appendix A. The minimal number of axes specifying completely the special stability groups is given. The vector specifies the direction of the axis and the fourth component its order. For the particular cases corresponding to C_2, a discussion is given in Appendix B together with the idea of the proof of the values of the parameters.

Stability group	Axes	A	A'	B	B'	C	C'	α	β	γ	Particular cases
$O(z)$	[(0,0,1)4] [(1,0,0)4]	0	0	0	0	0	0	γ	γ	γ	$\gamma=0$, SO(3)
$D_\infty(z)$	[(0,0,1)∞]	0	0	0	0	0	0	-4γ	-4γ	γ	$\gamma=0$, SO(3)
$D_4(z)$	[(0,0,1)4] [(1,0,0)2]	0	0	0	0	0	0	α	α	γ	$\alpha=\gamma$, cube $\alpha=-2\gamma$, cube $\alpha=-4\gamma$, D_∞
$D_3(z)$	[(0,0,1)3] [(1,0,0)2]	A	0	0	0	0	0	-4γ	-4γ	γ	$A^2=50\gamma^2$, cube $A=0$, D_∞
$D_3(d)$	[(1,1,1)3] [(1,−1,0)2]	A	A	A	A	A	A	γ	γ	γ	$A=0$, cube $10\gamma=13A$, cube $5\gamma=-7A$, D_∞
$D_2(z)$	[(0,0,1)2] [(1,0,0)2]	0	0	0	0	0	0	α	β	γ	$\alpha=\beta$, D_4 $\beta=\gamma$, D_4 $\alpha=\gamma$, D_4
$C_2(z)$	[(0,0,1)2]	0	0	0	0	C	C'	α	β	γ	See Appendix B D_2, D_3
$C_2(x)$	[(1,0,0)2]	A	A'	0	0	0	0	α	β	γ	See Appendix B D_2, D_3
$C_2(m)$	[(1,−1,0)2]	A	B	B	A	C	C	α	β	γ	See Appendix B D_2, D_3

1. SO(3) as stability groups

When all the parameters of S are zero, all the gradients in (3.27) are zero. All the extremality conditions are fulfilled, for all values of the potential coupling constants. The potential is zero. This extreme configuration is locally stable if μ is positive and clearly unstable if μ is negative (the more interesting case).

2. The group of the cube as stability groups

The nine equations in (3.37) are all linearly dependent. They reduce to

$$8\gamma^2(k + 15q) - 3p\gamma + 4\mu = 0 \tag{3.42}$$

up to an inessential factor 10γ, since γ is nonzero. Solutions of (3.42) exist provided

$$\Delta^2 = 9p^2 - 128\mu(k + 15q) > 0. \tag{3.43}$$

The asymptotic positivity condition (3.41) implies that (3.43) is fulfilled when μ is negative. When μ is positive p has to be sufficiently large.

The minimal potential assumes then the value

$$V_{(\text{cube})} = -\frac{15}{(k+15q)}\left(\mu^2 - \frac{3^2\mu p^2}{2^5(k+15q)} + \frac{3^3p^4}{2^{11}(k+15q)^2} + \frac{p\Delta^3}{2^{11}(k+15q)^2}\right), \tag{3.44}$$

where Δ is the positive square root of (3.43). (Remember that p is chosen positive.) The negative square root of (3.42) corresponds to a higher value of the potential.

3. D_∞ as stability group

Here also the nine equations in (3.37) are linearly dependent. They reduce to

$$16(8k+245q)\gamma^2 + 27p\gamma + 14\mu = 0 \tag{3.45}$$

up to a factor 10γ.

Solutions of (3.45) exist provided

$$\Omega^2 = (27p)^2 - 128\cdot 7\mu(8k+245q) > 0. \tag{3.46}$$

The minimal potential takes the value

$$V(D_\infty) = -\frac{245}{(8k+245q)}\left(\mu^2 - \frac{3^6\mu p^2}{2^5 7(8k+245q)} + \frac{3^{11}p^4}{2^{11}7^2(8k+245q)^2} + \frac{3^2p\Omega^3}{2^{11}7^2(8k+245q)^2}\right), \tag{3.47}$$

where Ω is the positive square root of (3.46).

Here again the negative square root of (3.46) corresponds to a higher value of the potential.

4. D_4 as stability group

Two of the nine equations (3.37) are linearly independent. Since

$$\alpha - \gamma = 0, \quad 3\alpha + 2\gamma = 0, \quad \alpha - 4\gamma = 0, \tag{3.48}$$

separately correspond to higher symmetries, these factors can be divided out leaving

$$3p - 16k\alpha = 0, \tag{3.49a}$$

$$\mu + 2q(9\alpha^2 + 2\alpha\gamma + 4\gamma^2) - 2k\alpha^2 = 0. \tag{3.49b}$$

The first equation fixes α while a solution for γ exists from the second provided

$$\mu < (9p^2/2^9k^2)(4k - 35q). \tag{3.50}$$

The potential takes the form

$$V(D_4) = \frac{5\cdot 3^4qp^4 - k(3^2p^2 - 2^7k\mu)^2}{2^{14}k^3q}. \tag{3.51}$$

5. D_3 as stability groups

Clearly all D_3's lead to the same relations, hence we work with $D_3(z)$. Only two of the nine equations (3.37) are linearly independent. Up to the nonzero factors these equations reduce to

$$p - 2k\gamma = 0, \tag{3.52a}$$

$$\mu + 8q(35\gamma^2 + 2A^2) + k(13\gamma^2 + A^2) = 0. \tag{3.52b}$$

Since $k + 16q$ is positive by the asymptotic positivity condition (3.41), the solution of (3.52b) for A exists if

$$\mu < -(280q + 13k)(p^2/4k^2). \tag{3.53}$$

For these values the Lagrangian becomes

$$V(D_3) = -\frac{16}{k+16q}\left(\mu^2 - \frac{9\mu p^2}{4k} - \frac{81p^4(k+20q)}{16k^3}\right). \tag{3.54}$$

6. D_2 as stability group

In the case D_2, which is completely symmetrical in α, β, γ, it is convenient to work with the symmetrized variables

$$\Sigma_1 = \alpha + \beta + \gamma, \quad \Sigma_2 = \alpha^2 + \beta^2 + \gamma^2, \quad \Sigma_3 = \alpha^3 + \beta^3 + \gamma^3. \tag{3.55}$$

There are three linearly independent equations in (3.37), hence one 3×3 determinant (3.38) has to be zero. This leads to the condition (when $\alpha \neq \beta \neq \gamma \neq \alpha$)

$$\Sigma_3 = \tfrac{1}{56}\Sigma_1(47\Sigma_1^2 - 39\Sigma_2). \tag{3.56}$$

The two remaining equations then become

$$\Sigma_1 = 3p/2k \tag{3.57}$$

and

$$\Sigma_2 = [-7\mu + \Sigma_1^2(2k - 7q)]/(3k + 49q). \tag{3.58}$$

The values α, β, and γ obeying (3.56)–(3.58) can be considered as the roots of a cubic equation with known coefficients. The condition for all roots to be real is

$$-18\Sigma_3^2 + 36\Sigma_1\Sigma_2\Sigma_3 - 8\Sigma_1\Sigma_3^3 + 3\Sigma_2^3 - 21\Sigma_1^2\Sigma_2^2 + 9\Sigma_1^4\Sigma_2 - \Sigma_1^6 > 0. \tag{3.59}$$

The value of the potential (3.28) is then

$$V(D_2) = [16k^3(3k+49q)]^{-1}[-784\mu^2k^3 + 1224\mu p^2k^2 + 81p^4(80q - k)]. \tag{3.60}$$

7. C_2 as stability group

The case can be worked out in complete detail. There are a number of solutions of Eqs. (3.37) of which only four are independent. After some algebra one obtains either D_2-type solutions, i.e.,

$$C = 0 \tag{3.61}$$

or

$$\alpha = \beta \tag{3.62}$$

or

$$\alpha + \beta + 8\gamma = 0 \tag{3.63}$$

or those of a D_3-type, i.e.,

$$-4C^2 + 4\gamma^2 - 8\alpha^2 - 8\beta^2 + (\alpha+\beta)\gamma - 15\alpha\beta = 0, \tag{3.64}$$

$$-48C^2\gamma + 104C^2(\alpha+\beta) - 24(\alpha^3+\beta^3) + 3\gamma(\alpha^2+\beta^2) - 101\alpha\beta(\alpha+\beta) - 6\alpha\beta\gamma = 0. \tag{3.65}$$

These equations can be found in Appendix B [Eqs. (B11)–(B14)] with x and z suitably interchanged. Hence there is no genuinely invariant C_2 minimum of the potential whatever may be the coupling constants.

8. The stability group reduced to the identity

In the general case when S has no nontrivial stability group Eqs. (3.37) depend fully on the six parameters. We

have not succeeded in solving analytically the determinants extracted from the matrix (3.38). We, however, feel that these equations are those implying that S corresponds to the symmetry D_2 at least. [See Appendix B, (f)]. Numerical explorations have confirmed this feeling.

E. Discussion of the results

We have so far obtained the analytical values of the extreme of the potential V for all allowed nontrivial subgroups of SO(3). These results now have to be studied as functions of the coupling constants μ, q, p, and k.

The problem can be considerably simplified by noting that by a suitable choice of scale for the fields and for the potential itself, two coupling constants (except q and k together) can be rescaled arbitrarily (see Appendix C). Since q is strictly positive (3.41), it can be rescaled to unity. On the other hand we have already stressed (3.28b) that p can be chosen to be positive. It is either zero or can be rescaled to unity. Hence the following two cases.

1. The $p=0$, $q=1$ case

This case is particularly simple. If μ is positive and the asymptotic condition is satisfied, none of the constraints (3.43), (3.46), (3.50), (3.53), and (3.59) is fulfilled. Hence and obviously the minimum of the potential is at S equal to zero and has SO(3) symmetry.

When μ is negative, all the conditions referred to above are satisfied, and all the potentials assume the simple form

$$V = -\mu^2(q+Rk)^{-1}, \tag{3.66}$$

where q is one and by order of increasing R,

$$R(D_4) = 0, \tag{3.67a}$$

$$R(D_\infty) = \tfrac{8}{245}, \tag{3.67b}$$

$$R(D_2) = \tfrac{3}{49}, \tag{3.67c}$$

$$R(D_3) = \tfrac{1}{16}, \tag{3.67d}$$

$$R(\text{cube}) = \tfrac{1}{13}. \tag{3.67e}$$

The stability group of the minimal configuration (lowest V) is the group of the cube when k is negative (but larger than $-15q$) and D_4 when k is positive. The stability groups D_∞, D_3, and D_2 never correspond to the absolute minimum. The case $k=0$ is highly degenerate since, as already noted, the accidental symmetry of the potential is O(9) and the stability group is O(8).

2. The case $p=1$, $q=1$

An analysis of the potentials when p and q equal unity shows that the absolute minimum of all the cases can only fall in one of the four categories according to their stability group SO(3), cube, D_∞, and D_4.

The best way to visualize the results is to plot in the k,μ plane ($k > -15$) the boundary between the regions with different stability groups. This is done in Fig. 1, where the qualitative behavior of the curves is given in a compactified plot of the relevant half of the k,μ plane ($k=[-15,\infty]$, $\mu=[-\infty,+\infty]$). As is seen there are three triple points T_1, T_2, and T_3 whose coordinates are given in the figure caption together with the coordinates of other convenient points.

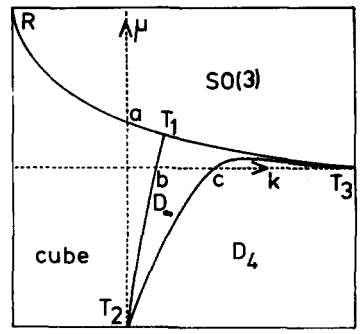

FIG. 1. Phase diagram for the absolute minimum in the $s=4$ case as a function of the coupling constants. The coupling constants q and p are rescaled to the value unity (see Appendix C). Useful coordinates: the triple points, $T_1=(20,\frac{1}{360})$, $T_2=(0,-\infty)$, $T_3=(\infty,0)$; the asymptotic point, $R=(-15,\infty)$; the crossing points with the coordinate axis, $a=(0,\frac{1}{240})$, $b=(5(7^2-3^{10/3})/(3^{7/3}-8),0)$, $c=(245,0)$.

It should be stressed that the triple points always involve the D_∞ region.

The curve between T_1 and R has the form

$$\mu = [16(k+15)]^{-1}. \tag{3.68}$$

The curve between T_1 and T_3 has the form

$$\mu = 3^4/(2^47(8k+245)). \tag{3.69}$$

The two curves between T_2 and T_3 and between T_2 and T_1 have a much more complicated expression. For example, the boundary curve between D_∞ and D_4 can be represented implicitly by a polynomial of fourth degree in μ and of the 12th degree in k. For these reasons, we refrain from presenting here the exact form, prefering to give some asymptotic formula. Near the coordinate axes, we have, respectively,

$$T_1 - T_2: \quad k^2\mu = -0.723, \quad \text{for } k\to 0, \tag{3.70}$$

$$T_2 - C: \quad k^2\mu = -12.18, \quad \text{for } k\to 0, \tag{3.71}$$

$$C - T_3: \quad k\mu = \tfrac{9}{128}, \quad \text{for } k\to\infty. \tag{3.72}$$

This completes the description of the phase diagram.

Let us finish this section with a few remarks.

(i) The case $p=0$ (1) can be recovered as the limit of the case $p=1$ (2) when μ goes to plus or minus infinity; this is obvious in view of formula (C4a) since the choice

$$q=\tilde{q}=p=1=\pm\tilde{\mu} \tag{3.73}$$

leads to the connection

$$\mu = \pm 1/\tilde{p}^2. \tag{3.74}$$

When $\tilde{p}$ in one plot goes to zero, μ in the other plot goes to infinity.

(ii) The group D_4 [which is not maximal in SO(3) for $s=4$], appears to be the stability group of the absolute minimum of V for quite a large region of the coupling constant space. This seems to us an interesting contribution in the literature developed around Michel's conjecture.

(iii) Despite our initial hopes we have found no region corresponding to configurations invariant under D_2 or D_3 or with no invariance except the identity and giving an absolute minimum of the potential.

(iv) Contrary to our expectations based on formula (3.39), (3.40), there is no boundary (see Fig. 1) between the D_4 phase and the cube phase, except at the triple point T_2.

IV. CONCLUSIONS

In this paper, we have analyzed in complete detail and as a function of the coupling constants all the absolute minima of the most general Landau potential in the framework of one irreducible representation of spin up to 4 of SO(3). We have concentrated most of our attention on the stability group of the minimal configurations.

For s equal to 1 and 2, the known results have been recovered and were presented for the purpose of completeness. The s equals 3 case is in agreement with the expectations: only configurations with maximal stability groups appear as absolute minima.

The case s equals 4 is richer. The results are summarized in Fig. 1 where the regions corresponding to the allowed stability groups of absolute minima configurations are drawn as a function of two coupling constants.

It is to be stressed that the nonmaximal subgroup D_4 has an important region associated to it while D_2 and D_3 never appear. This we find an interesting contribution to the literature about Michel's conjecture.

We have also presented in Sec. II F a systematic way to put any configuration in canonical position using the freedom of an arbitrary SO(3) transformation. This idea can easily be extended to other continuous symmetry groups.

Finally, we want to highlight our Eq. (2.12) which allows the computation of the possible axis of symmetry of a given configuration for any irreducible representation of SO(3) as a generalized (nonlinear) eigenvalue equation.

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APPENDIX A: SUBGROUPS OF SO(3)

In this appendix let us recall some well-known results concerning the relevant subgroups of SO(3). Apart from the (trivial) subgroup E reduced to the identity we list and denote the following.

1. The C subgroups

The subgroup $C_n(a)$ is defined by the n rotation of angles $2\pi k/n$ $(k=0,1,\ldots,n-1)$ (including the identity) around a fixed axis (a). Its order is n.

2. The D subgroups

The subgroup $D_n(a)$ is generated by the n rotations of the group $C_n(a)$, together with one rotation of π, $C_2(b)$, around one axis (b) orthogonal to (a). Its order is $2n$. Hence there are n subgroups $C_2(b_i)$. All (b_i)'s are orthogonal to (a) and the angle between (b_i) and (b_{i+1}) is equal to π/n.

3. The $C_\infty(a)$ subgroups

The subgroup $C_\infty(a)$ is the SO(2) rotation group around an axis (a).

4. The $D_\infty(a)$ subgroups

The subgroup $D_\infty(a)$ is generated by an SO(2) subgroup and a $C_2(b)$ around one axis (b) orthogonal to (a). [Hence there is a $C_2(b)$ around any axis (b) orthogonal to (a).]

5. The tetrahedron group T

The elements of the tetrahedron group are generated by the elements of the four C_3 groups with the axis joining the summits of a regular tetrahedron to the center of the opposite face and the three C_2 groups with the axis joining the middle of opposite edges of the tetrahedron. Its order is 12.

6. The cube group O

The group of the cube has three C_4 subgroups with the axis joining the center of opposite faces, four C_3 subgroups with the axis joining opposite summits, and six C_2 subgroups with the axis joining the middle of opposite edges of the cube. Its order is 24 (it obviously has also D-type subgroups).

7. The dodecahedron or icosahedron group Y

The icosahedron is a regular polyhedron with 20 equilateral triangular faces, 12 summits, and 30 edges. The C_5 subgroups are associated to the six axes joining opposite summits; the C_3 subgroups are associated to the ten-axis joining opposite center of faces; and the C_2 subgroups are associated to the axis joining opposite edges. Its order is 60.

In general the order is given by

$$\text{order} = \sum_{(a)} p_a (n_a - 1) + 1,$$

where p_a is the number of axes with C subgroups of order n_a.

APPENDIX B: SO(2) DECOMPOSITION OF $s=4$ CONFIGURATIONS. PARAMETER RESTRICTIONS

As is well known the spin s irreducible representation of SO(3) is decomposed under an SO(2) subgroup in one singlet and s real doublets. Each one transforms with angle $k\theta$ $(k=1,\ldots,s)$ according to

$$d_k^T = \begin{pmatrix} \cos k\theta & \sin k\theta \\ -\sin k\theta & \cos k\theta \end{pmatrix} d_k. \tag{B1}$$

If one asks for the configuration invariant under $C(a)$ of order p, all the doublets of type k, such that the quotient of k by p is not an integer n, must obviously be zero.

On the other hand if $d^{(1)}$ and $d^{(2)}$ are the components of d, define

$$d_k^+ = d_k^{(1)} - i d_k^{(2)}, \quad d_k^- = d_k^{(1)} + i d_k^{(2)}. \tag{B2}$$

They transform as

$$d_k^{+T} = e^{ik\theta} d_k^+, \quad d_k^{-T} = e^{-ik\theta} d_k^-, \tag{B3}$$

and are one-dimensional complex representations. Hence we find the SO(2) invariants, the length squared

$$I_k^2 = d_k^+ d_k^- = d_k^{(1)2} + d_k^{(2)2}, \tag{B4}$$

and, more generally, the multiple products

$$d_{k_1}^+ d_{k_2}^+ \cdots d_{k_r}^+ d_{k_{r+1}}^- d_{k_{r+2}}^- d_{k_{r+s}}^-, \qquad \sum_{i=1}^{r} k_i = \sum_{i=r+1}^{s} k_i . \tag{B5}$$

As an application of these ideas let us give and prove some of the results of Table IV for $s = 4$. The notation is that of Table IV.

(a) The SO(2) rotation group around the z axis decomposes S as follows [see (3.29) and (3.30) for notation]:

$$d_0 = \alpha + \beta, \quad d_1 = \begin{pmatrix} B \\ A' \end{pmatrix}, \quad d_2 = \begin{pmatrix} \alpha - \beta \\ 2(C + C') \end{pmatrix}, \qquad d_3 = \begin{pmatrix} 4A + 3A' \\ 4B' + 3B \end{pmatrix}, \quad d_4 = \begin{pmatrix} 4(C - C') \\ \alpha + \beta + 8\gamma \end{pmatrix}. \tag{B6}$$

Under SO(2) with axis $(1, -1, 0)$ one has instead

$$d_0 = 4C + 4C' + \alpha + \beta - 4\gamma,$$
$$d_1 = \begin{pmatrix} 4A + 6A' - 6B - 4B' \\ -(2C - 2C' - \alpha + \beta)2^{1/2} \end{pmatrix},$$
$$d_2 = \begin{pmatrix} 8A + 4A' + 4B + 8B' \\ -(4C + 4C' + 3\alpha + \beta + 4\gamma)2^{1/2} \end{pmatrix}, \tag{B7}$$
$$d_3 = \begin{pmatrix} 12A + 2A' - 2B - 12B' \\ -(2C - 2C' + 7\alpha - 7\beta)2^{1/2} \end{pmatrix},$$
$$d_4 = \begin{pmatrix} 16A + 40A' + 40B + 16B' \\ -(28C + 28C' - 77\alpha - 17\beta + 4\gamma)2^{1/2} \end{pmatrix}.$$

(b) If one wants $C_2(z)$, d_1 and d_3 in (B6) must be zero, hence

$$C_2(z): \quad A = A' = B = B' = 0. \tag{B8}$$

Moreover by a suitable rotation the first component of d_4 may be brought to zero, hence

$$C = C', \tag{B9}$$

i.e., a canonical position.

(c) If one wants $C_4(z)$, d_1, d_2, and d_3 in (B6) must be zero, hence

$$C_4(z): \quad A = A' = B = B' = 0, \qquad \alpha = \beta, \qquad C = -C'. \tag{B10}$$

Moreover by a suitable rotation the first component of d_4 may be brought to zero. Hence

$$C = C' = 0, \tag{B11}$$

i.e., a canonical position.

It should be remarked that this position is automatically $C_2(x)$ invariant and hence $D_4(z)$.

(d) As an example let us give the restrictions imposed on the parameters of $C_2(x)$ to be a D_3. The quantities invariant under $C_2(x)$ must be equal to those of a D_3. After some algebra one obtains the two relations

$$-4A^2 + 4\alpha^2 - 8\beta^2 - 8\gamma^2 + \alpha\beta + \alpha\gamma - 15\beta\gamma = 0,$$
$$-48A^2\alpha + 104A^2\gamma + 104A^2\beta - 24\beta^3 - 24\gamma^3 + 3\alpha\gamma^2 + 3\alpha\beta^2 - 101\beta\gamma^2 - 101\beta^2\gamma - 6\alpha\beta\gamma = 0, \tag{B12}$$

by eliminating the two arbitrary parameters of D_3.

(e) The restrictions imposed on the parameters of $C_2(x)$ to be a D_2 can also be found using the same technique. The invariant of $C_2(x)$ must be those of a D_2. After some algebra one obtains three possibilities for the parameters. Either

$$A = 0 \tag{B13}$$

or

$$\beta = \gamma \tag{B14}$$

or

$$8\alpha + \beta + \gamma = 0. \tag{B15}$$

(f) Relations involving the axis $m(1, -1, 0)$ instead of z can be analogously obtained from (B7) instead of (B6).

Finally we end this appendix by noting that the restrictions on the parameters of a general canonical position, which imply C_2 (or D_2) invariance, can be obtained in the following way.

There are six independent SO(3) invariants (of the six canonical parameters S). When the configuration is C_2 (resp. D_2) invariant it depends only on four (resp. three) canonical parameters S' as do the invariants. Equating the invariants for S and S' and eliminating the four (resp. three) S', two (resp. three) relations remain among the S parameters. These are the relations which guarantee C_2 (resp. D_2) invariance. We have not tried to write these relations explicitly.

APPENDIX C: RESCALING

Let S be the fields and V the potential. Clearly

$$V = \rho\tilde{V} \quad (\rho > 0), \tag{C1}$$
$$S = \lambda\tilde{S}, \tag{C2}$$

correspond to essentially the same configuration rescaled. Hence the new coupling constants are related to the old ones by

$$\mu\lambda^2 = \rho\tilde{\mu}, \tag{C3a}$$
$$q\lambda^4 = \rho\tilde{q}, \tag{C3b}$$
$$p\lambda^3 = \rho\tilde{p}, \tag{C3c}$$
$$k\lambda^4 = \rho\tilde{k}. \tag{C3d}$$

Eliminating ρ and λ the arbitrary scales leads to the conserved quantities

$$p^2/q\mu = \tilde{p}^2/\tilde{q}\tilde{\mu}, \tag{C4a}$$
$$k/q = \tilde{k}/\tilde{q}. \tag{C4b}$$

Since by the asymptotic positivity condition (3.41) q is positive, it can be rescaled to unity, by adjusting k [see (C4b)], without losing any generality. By the same argument using (C4a) p can be rescaled to be zero or unity by adjusting μ and the sign of S.

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Long-range dynamics and broken symmetries in gauge models. The Schwinger model

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The occurrence of variables at infinity in the dynamics of gauge models (in positive gauges) as a result of the Coulomb-type interaction is rigorously shown in two-dimensional quantum electrodynamics, in the Coulomb gauge. The general structures associated to the algebraic dynamics of systems with long-range interactions, like the removal of the infrared cutoff, the effective dynamics, the classical motion of the variables at infinity, and their relevance for the generalization of the Goldstone theorem and the spectrum of the generalized Goldstone bosons, are explicitly shown in this model; in particular, the chiral symmetry breaking and the associated mass generation is discussed in detail. The analogous results for the chiral Schwinger model are briefly summarized.

I. FORMAL DEFINITION OF THE MODEL IN THE BOSONIZED FORM IN THE COULOMB GAUGE. GENERAL PROBLEMS

The Schwinger model describes two-dimensional quantum electrodynamics (QED_2) and it is formally defined by the following Lagrangian[1]:

$$\mathscr{L} = \int dx\left(\bar{\psi} i \partial\!\!\!/ \psi - g\bar{\psi} A\!\!\!/ \psi - \frac{1}{4}F_{\mu\nu}F^{\mu\nu}\right). \tag{1.1}$$

In the Coulomb gauge one has

$$\partial_1 A_1 = 0$$

and one chooses

$$A_1 = 0.$$

The Maxwell equations then give

$$\partial_1^2 A_0 = g\psi^\dagger\psi$$

and

$$A_0(x) = \frac{1}{2}g\int |x-x'|\psi^\dagger(x')\psi(x')dx' . \tag{1.2}$$

The formal Lagrangian then becomes ($V(x) \equiv \frac{1}{2}|x|$)

$$\mathscr{L} = \int dx(\bar{\psi} i \partial\!\!\!/ \psi) + \frac{1}{4}\int dx\, dx'\, \psi^\dagger(x)\psi(x) \times V(x-x')\psi^\dagger(x')\psi(x') .$$

The Lagrangian further simplifies if one adopts fermion bosonization, namely the remarkable property that in one space dimension a fermion system can be described by a bosonic field. The basic correspondence is[2]

$$\begin{aligned} &j_\mu = \bar{\psi}\gamma_\mu\psi = (1/\sqrt{\pi})\epsilon_{\mu\nu}\partial^\nu\varphi , \\ &j_\mu^5 = \bar{\psi}\gamma_\mu\gamma_5\psi = (1/\sqrt{\pi})\partial_\mu\varphi , \\ &\bar{\psi}\psi = K{:}\cos 2\sqrt{\pi}\varphi{:}, \quad \bar{\psi}\gamma_5\psi = K{:}\sin 2\sqrt{\pi}\varphi{:} , \\ &i\bar{\psi}\,\partial\!\!\!/\psi = \tfrac{1}{2}\partial_\mu\varphi\,\partial^\mu\varphi, \quad K = \text{const} . \end{aligned} \tag{1.3}$$

If the fermion is massless, so is also the boson, as follows clearly from the last equation, which relates the two Lagrangians. (It also follows from the conservation of j_μ and j_μ^5 and the relation $j_\mu = \epsilon_{\mu\nu}j^{5\nu}$.) The boson field is also a canonical field since the current commutation relation

$$[j_0(x), j_1(x')] = (-i/\pi)\delta'(x-x')$$

implies the CCR for φ:

$$[\varphi(x), \dot{\varphi}(x')] = i\delta(x-x') .$$

For a rigorous discussion of the boson–fermion correspondence see Ref. 3, Sec. 6C, and references therein.

In the bosonized form the Lagrangian then takes the form

$$\mathscr{L} = \frac{1}{2}\int [\dot{\varphi}^2 - (\partial_1\varphi)^2]dx + \frac{1}{4}\frac{g^2}{\pi}\int \partial_1\varphi(x)|x-x'|\partial_1\varphi(x')dx\,dx' ,$$

which yields the following formal Hamiltonian:

$$H = \frac{1}{2}\int [\pi^2 + (\partial_1\varphi)^2]dx - \frac{e^2}{4}\int \partial_1\varphi(x)\partial_1\varphi(y)|x-y|dx\,dy , \tag{1.4}$$

where $\pi = \dot{\varphi}$ is the canonical momentum conjugate to φ, and $e^2 \equiv g^2/\pi$.

In the standard treatment of the model[4,5] one then argues that in discussing the (representation of the) field φ one is naturally led to the introduction of an "angle" θ and its conjugate variable Π_θ, which should in some way specify the boundary conditions at infinity. Then Π_θ is recognized to be the generator of chiral transformations and the ground state degeneracy with respect to chiral transformations is then interpreted in terms of chiral breaking (θ vacua and chiral breaking) without associated Goldstone bosons.

A pedantic look at the literature, however, leaves several questions of principle unsettled or unclear.

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(i) If θ has the meaning of $\lim_{x\to\infty}\varphi(x)\equiv\varphi_\infty$, then it should belong to the commutant of the algebra generated by φ and π, and the introduction of a momentum $\Pi_\theta=\pi_\infty$ conjugated to φ_∞ is problematic if one considers representations with time translation invariance.

(ii) In some of the discussions, the appearance of the angle θ seems to be strictly related to the fermion bosonization and therefore the ensuing mechanism of θ vacua, chiral symmetry breaking, and mass generation appears to be linked to the two-dimensional case.

(iii) From a more general point of view the occurrence of inequivalent representations of the algebra generated by φ and π and their characterization in terms of the algebra of local observables does not seem obvious in terms of the dynamics defined by the Hamiltonian (1.4).

(iv) The model has been regarded as a prototype of chiral symmetry breaking without Goldstone bosons and as such it should suggest a general mechanism for the field theoretical solution of the U(1) problem in four dimensions, but there does not seem to be complete agreement in the literature about the identification of such a mechanism ("seizing of the vacuum," "chiral anomaly," etc.).

In view of the above remarks it seems necessary to have a rigorous control of the model so that one can identify general mathematical structures and/or mechanisms with a much more general validity than in the two-dimensional case.[4] In particular, we will show the following.

(a) The long-range interaction leads to the occurrence of "variables at infinity" in the time evolution of local variables and in this respect the model provides a nontrivial example of the general structures discussed in Refs. 6–8 (the model is not a mean field model!).[9]

(b) The model exhibits in a clear way the mechanism of a generalized Goldstone theorem by which the generalized Goldstone bosons have a nonzero mass generated by the nontrivial "classical motion" of the variables at infinity. In this sense our treatment provides a rigorous meaning (and understanding) of the so-called mechanism of "seizing of the vacuum."[4]

(c) The model exhibits mathematical structures and properties in strong analogy with the Stückelberg–Kibble model[6,7,10,11] and the Coulomb gas (with uniform background).[12]

(d) From a more mathematical point of view the model provides a prototype of a field theory in which the long-range interaction requires to abandon the local algebraic framework of Haag and Kastler in favor of a more general structure, and it suggests that this may in fact be the case in gauge quantum field theories, in positive gauges. In particular, the model shows that the algebraic time evolution of the *observable* algebra involves variables at infinity.

II. ALGEBRA OF CANONICAL VARIABLES (WEYL ALGEBRA). QUASIFREE STATES

We start by introducing an algebraic setting on which an infrared cutoff dynamics will be defined; we will then consider the removal of the infrared cutoff and discuss the resulting mathematical structures along the lines of Ref. 6.

The basic (local) algebra $\mathscr{A}$ is that generated by the canonical variables $\varphi(f)$, $\pi(g)$, $f,g\in\mathscr{S}_{\rm real}(R^s)$, $s=$ space dimensions, obeying the canonical commutation relations (CCR's)

$$[\pi(g),\varphi(f)]=-i\int d^sx\,g(x)f(x)\equiv -i(g,f)\,. \tag{2.1}$$

Following the standard procedure,[13] it is convenient to introduce the linear space $\mathscr{F}=\mathscr{S}_{\rm real}(R^s)\times\mathscr{S}_{\rm real}(R^s)$ of pairs $F=(f_1,f_2)$ and the Weyl operators $W(F)$, with the properties

$$\begin{aligned} &W(F)^*=W(-F)\,,\\ &W(F)W(G)=W(F+G)\exp[-(i/2)\langle F,G\rangle]\,, \end{aligned} \tag{2.2}$$

where $\langle\cdot,\cdot\rangle$ is the symplectic form on $\mathscr{F}$ defined by the CCR:

$$\begin{aligned} &[\Phi(F),\Phi(G)]=i\langle F,G\rangle=i[(f_1,g_2)-(f_2,g_1)]\,,\\ &\Phi(F)\equiv\varphi(f_1)+\pi(f_2)\,. \end{aligned} \tag{2.3}$$

The Weyl operators generate a unique abstract C^* algebra $\mathscr{A}$ (*Weyl* algebra) (see Ref. 13, Theorem 5.2.8, p. 20). This (equal time field) algebra $\mathscr{A}$ is well defined also in one space dimension; the problems associated to the infrared singularities will emerge at the level of the definition of the dynamics in the limit of no infrared cutoff, of the existence of a ground state, as well as the regularity[14] of the representation of $\mathscr{A}$, so that one may (or may not) recover the fields φ,π from the Weyl operators.

For the following it will be useful to recall that[13] any linear invertible transformation T defined on $\mathscr{F}$, which preserve the symplectic form:

$$\langle T(F),T(G)\rangle=\langle F,G\rangle \tag{2.4}$$

defines a unique automorphism α_T of $\mathscr{A}$

$$\alpha_T(W(F))=W(T(F))\,. \tag{2.5}$$

For the following, in order to remove the infrared cutoff in the dynamics, according to the general framework of Ref. 6, one has to make reference to a family $\mathbb{F}$ of (physically) relevant states. To this purpose, since the Hamiltonian (1.4) defines a linear dynamics, it is reasonable to consider the family of quasifree states on $\mathscr{A}$. They are characterized by the factorization of the n-point functions into sums of products of two point functions and therefore by the following expectation:

$$\omega(W(F))=\exp(-\tfrac{1}{4}[F,F])\,, \tag{2.6}$$

where $[\cdot,\cdot]$ is a (positive) majorant of the CCR symplectic form

$$|\langle F,G\rangle|^2\leqslant[F,F][G,G],\quad [F,F]\geqslant 0\,. \tag{2.7}$$

Furthermore, if

$$[F,G]=-\langle F,JG\rangle\,, \tag{2.8}$$

with J defined on a dense domain of $\mathscr{F}\equiv\mathscr{S}_{\rm real}\times\mathscr{S}_{\rm real}$, dense with respect to the topology defined by $[\cdot,\cdot]$, and such that

$$J^2=-1, \tag{2.9}$$

then ω is a pure state.

This structure is usually classified in terms of a complex

scalar product: in fact, given a real scalar product $[\cdot,\cdot]$ on $\mathcal{F}$ satisfying (2.7) and (2.8) one can introduce a complex structure in the following way defining:

$$[F,G]_c \equiv [F,G] + i\langle F,G\rangle \tag{2.10}$$

and, for any complex λ,

$$\lambda F \equiv (\mathrm{Re}\,\lambda)F + (\mathrm{Im}\,\lambda)JF, \tag{2.11}$$

one gets that $[\cdot,\cdot]_c$ is a sesquilinear scalar product on $\mathcal{F}$, where the complexification of $\mathcal{F}$ is given by (2.11). Conversely, given a complex structure $[\cdot,\cdot]_c$ on $\mathcal{F}$ one can recover an operator J, with $J^2 = -1$ such that Eqs. (2.10), (2.11), and (2.8) hold.

Since the symplectic form is given by the CCR's, the classification of the pure quasifree states is reduced to the classification of the real operators J (densely defined) on $\mathcal{F}$ such that

$$J^2 = -1, \quad -\langle F,JG\rangle = \text{positive symmetric form}. \tag{2.12}$$

In the following we will further restrict our attention to translationally invariant states ω (and to the corresponding GNS representations). The translational invariance of $[F,G] = -\langle F,JG\rangle$ then requires

$$(JF)_i(x) = \int d^s y\, J_{ij}(x-y) f_j(y), \quad i = 1,2. \tag{2.13}$$

Proposition 2.1: The real operators J satisfying (2.12) and (2.13) are characterized by matrices (in k space) of the form

$$\tilde{J}(k) = \begin{pmatrix} \alpha(k) & r(k)(1+\alpha^2(k))^{1/2} \\ -(1+\alpha^2(k))^{1/2}/r(k) & -\alpha(k) \end{pmatrix}, \tag{2.14}$$

with α real and $r > 0$.

Proof: Conditions (2.12) and (2.13) imply

$$J_{ij}(x) = J_{ij}(-x), \quad i \neq j, \quad J_{11}(-x) = -J_{22}(x). \tag{2.15}$$

The condition $J^2 = -1$ then gives

$$\tilde{J}(k) = \begin{pmatrix} \alpha & \beta \\ \gamma & -\bar{\alpha} \end{pmatrix}, \quad \beta\gamma = -(1+\alpha^2), \tag{2.16}$$

β,γ real and α real if β or γ does not vanish.

Furthermore, the positivity condition (2.12):

$$-\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} J > 0$$

by Eq. (2.16) is equivalent to

$$(1+\alpha^2)/\beta + \beta > 0, \quad \text{i.e.,} \quad \beta > 0.$$

Letting $r \equiv \beta(1+\alpha^2)^{-1/2}$, one gets the form (2.14); this completes the proof.

Given an operator J, with $J^2 = -1$ and $-\langle F,JF\rangle > 0$, $\forall F$, by Eq. (2.8) one may then define a real scalar product $[\cdot,\cdot]$ on $\mathcal{F}$ and its extension to a sesquilinear form by Eq. (2.10).

For the following it is convenient to characterize the scalar product $[\cdot,\cdot]$ in terms of a matrix $M_{ij}(k)$

$$[F,G] = \sum_{i,j} \int d^s k\, \bar{f}_i(k) M_{ij}(k) g_j(k) \equiv [F,G]_M, \tag{2.17}$$

$$M = -\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} J = \begin{pmatrix} (1+\alpha^2)^{1/2} r^{-1} & \alpha \\ \alpha & (1+\alpha^2)^{1/2} r \end{pmatrix}. \tag{2.18}$$

The corresponding state, defined by Eq. (2.6), will then be denoted by ω_M. A simple extension of the states ω_M is given by the states

$$\omega_{M,\lambda}(W(F)) = \omega_M(W(F)) e^{i\lambda \tilde{f}_1(0)}, \quad \lambda \in \mathbf{R} \tag{2.19}$$

(they define representations with a nonvanishing expectation value of the field φ, $\langle\varphi\rangle = \lambda$).

III. INFRARED CUTOFFED DYNAMICS. CHIRAL SYMMETRY

To give a meaning to the formal Hamiltonian (1.4) and to define the time evolution on $\mathcal{A}$ one has to introduce an infrared cutoff; to this purpose we will replace the long-range potential $|x|/2$ by

$$V_L(x) \equiv \tfrac{1}{2}|x| f_L(x), \tag{3.1}$$

where $f_L(x) = f(|x|/L)$, $f \in \mathcal{D}(R^1)$, $f(x) = 1$ for $|x| < 1$, $f(x) = 0$ for $|x| > 1 + a$. Strictly speaking, one should also introduce an infrared cutoff in the kinetic terms and a Wick ordering, in order to define a regularized time evolution α_L^t on $\mathcal{A}$ by[15]

$$\alpha_L^t(A) = e^{iH_L t} A e^{-iH_L t}, \quad \forall A \in \mathcal{A}. \tag{3.2}$$

The infrared cutoff on the kinetic terms can be easily removed in the equations of motion (and therefore it is not strictly necessary) and the Wick ordering subtraction is irrelevant for Eq. (3.2).[16]

The resulting equations of motion are

$$\begin{aligned} &\dot{\varphi}(f) = \pi(f), \\ &\dot{\pi}(g) = \varphi(\Delta g - e^2 g + e^2 \sigma_L * g), \end{aligned} \tag{3.3}$$

where

$$\sigma_L(y) = -\Delta(f_L(y)|y|/2) + \delta(y) \tag{3.4}$$

[and therefore $\int \sigma_L(y)dy = 1$, $\sigma_L(y) = \sigma_L(-y)$, $\mathrm{supp}\,\sigma_L \subset \{y: L < |y| < L(1+a)\}$].

Equations (3.3) can be easily integrated and yield [in the notations of Eq. (2.3)]

$$\Phi_t(F) = \Phi(F_t), \tag{3.5}$$

where

$$\tilde{F}_t(k) = \tilde{A}_L^t(k)\tilde{F}(k), \tag{3.6}$$

$$\tilde{A}_L^t = \begin{pmatrix} \cos\omega_L t & -\omega_L \sin\omega_L t \\ \omega_L^{-1}\sin\omega_L t & \cos\omega_L t \end{pmatrix}, \tag{3.7}$$

$$\omega_L^2 \equiv k^2(1 + \tilde{V}_L(k)).$$

[Note that, since $\tilde{\sigma}_L(0) = 1$, one has $\omega_L(0) = 0$.] Since the elements of $\tilde{A}_L^t$ are C^∞ even functions of $\omega_L(k)$, which are bounded by polynomials in k, and $\omega_L^2(k)$ is a C^∞ function of k, A_L^t defines a mapping of $\mathcal{F} = \mathcal{S} \times \mathcal{S}$ into itself.

Furthermore, one can easily check that the mapping (3.6) leaves the symplectic form (2.3) invariant:

$$(\overline{A^t_L}(k))^T\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}A^t_L(k)=\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix},$$

T = transpose,

and therefore, according to Eqs. (2.4) and (2.5), it defines an *automorphism* of $\mathscr{A}$

$$\alpha^t_L(W(F))\equiv W(A^t_L F)\equiv W(F^t_L) \tag{3.8}$$

(*infrared cutoffed dynamics*).

Another obvious automorphism of $\mathscr{A}$ is that corresponding to *the shift of the field* φ

$$\beta^\lambda:\ \varphi\to\varphi+\lambda,\quad \pi\to\pi\,. \tag{3.9}$$

More precisely, the mapping

$$\beta^\lambda(W(F))=W(F)\exp\left[i\lambda\int dx f_1(x)\right], \tag{3.10}$$

where $F=(f_1,f_2)\in\mathscr{F}$, leaves the algebraic structure of the CCR's, Eqs. (2.2) [or Eqs. (2.3)], invariant and therefore it defines an automorphism of $\mathscr{A}$. Furthermore, one has

$$\beta^\lambda\alpha^t_L=\alpha^t_L\beta^\lambda\,, \tag{3.11}$$

since, by Eqs. (3.7), $\tilde f^t_1(0)=\tilde f_1(0)$. From the equations which define the fermion bosonization it follows that β^λ corresponds to chiral transformations and therefore by Eq. (3.11) the infrared cutoffed dynamics has *chiral symmetry*.

IV. PHYSICALLY RELEVANT STATES AND REMOVAL OF THE INFRARED CUTOFF IN THE DYNAMICS

The long range of the interaction prevents the existence of the limit $L\to\infty$ of α^t_L in the norm topology and therefore, according to the general discussion of Ref. 6, the removal of the infrared cutoff requires to make reference to (the weak topology defined by) a family of "physically relevant" states, sufficiently regular at infinity. We will consider a family $\mathbb{F}$ of states of the form discussed in Sec. II. The following proposition makes clear the regularity conditions at (space) infinity which allow the strong convergence of α^t_L.

Proposition 4.1: Let $\mathbb{F}$ be the family of states of the form (2.19)

$$\omega_{M,\lambda}(W(F))=\exp(-\tfrac{1}{4}[F,F]_M+i\lambda\tilde f_1(0))\,, \tag{4.1}$$

with the matrix $M_{ij}(k)$ satisfying

$$M_{11}(k),M_{22}(k)\in L^1_{\rm loc} \tag{4.2}$$

(i.e., locally in L^1 and bounded by polynomials for large k's),[17] then the following holds.

(A) α^t_L is convergent in the strong topology defined by the states $\hat{\mathbb{F}}$ of the (quasifree) representations defined by (4.1).

(B) The (weak) convergence of α^t_L defines a mapping $\lim_{L\to\infty}(\alpha^t_L)^*=(\alpha^t)^*$ of $\hat{\mathbb{F}}$ into the dual $\mathscr{A}'$ with the property that

$$(\alpha^t)^*\hat{\mathbb{F}}\subset\hat{\mathbb{F}} \tag{4.3}$$

and $(\alpha^t)^*$ defines a one-parameter group

$$(\alpha^{t_1})^*(\alpha^{t_2})^*=(\alpha^{t_1+t_2})^*\,. \tag{4.4}$$

(C) Hence $(\alpha^t)^*$ uniquely determines a one-parameter group α^t, $t\in\mathbb{R}$, of automorphisms of $\mathscr{M}=\overline{\mathscr{A}}$, where the bar denotes the weak closure with respect to the (weak) topology induced by the states of $\hat{\mathbb{F}}$.[18]

For the proof see the Appendix.

We may now explicitly identify the algebraic dynamics α^t obtained by removing the infrared cutoff. To this purpose we remark that, since $\tilde f^t_{1,L}(0)=\tilde f_1(0)$,

$$\begin{aligned}&\lim_{L\to\infty}\lim_{k\to 0}\tilde f^t_{1,L}(k)\\ &\quad=\tilde f_1(0)\neq\lim_{k\to 0}\tilde f^t_1(k)\\ &\quad=\lim_{k\to 0}\left[(\cos\omega(k)t)\tilde f_1(k)+\omega(k)^{-1}\sin\omega(k)t\tilde f_2(k)\right]\\ &\quad=\cos\omega_0 t\tilde f_1(0)+\omega_0^{-1}\sin\omega_0 t\tilde f_2(0)\equiv\tilde f^t_1(0)\,,\end{aligned} \tag{4.5}$$

where $\omega(k)\equiv\omega_\infty(k)$, $\omega_0\equiv\omega(0)$, and therefore from the proof of (A) in the Appendix it follows that in each representation $\Pi_{M,\lambda}$ defined by $\omega_{M,\lambda}$,

$$\begin{aligned}&\Pi_{M,\lambda}(\alpha^t_L W(F))\\ &\quad\to\Pi_{M,\lambda}(\alpha^t W(F))\\ &\quad=\Pi_{M,\lambda}(W(F^t))\exp\left[i\lambda(\tilde f_1(0)-\tilde f^t_1(0))\right]\,.\end{aligned} \tag{4.6}$$

V. ALGEBRAIC DYNAMICS AND VARIABLES AT INFINITY. EFFECTIVE DYNAMICS

One might wonder whether the careful analysis of the previous section is really necessary or it is somewhat academic. As a matter of fact, the removal of the infrared cutoff requires special care, especially from the mathematical point of view, and in any case one wants a rigorous control on the controversial treatments appeared in the literature,[4,5] and a clear understanding of the so-called "seizing of the vacuum." One of the crucial issues is how a formally symmetric Hamiltonian [Eq. (1.4) or in the regularized form (3.1)] may lead to asymmetric equations; as we will see the careful removal of the infrared cutoff leads to an algebraic dynamics α^t that is symmetric, does not leave the canonical local algebra $\mathscr{A}$ stable, and requires the introduction of variables at infinity. Furthermore, in some of the discussions in the literature the introduction of the θ angle is somewhat related to the "value of the field φ at infinity."[19]

In order to make the above points precise, we start by identifying the *variable at infinity associated to* φ. Let $F_n\equiv(f_{1n},0)$, with $\tilde f_{1,n}(0)=1$, $\forall n$ and such that[20]

$$\lim_{n\to\infty}[F_n,F_n]_M=0\,, \tag{5.1}$$

for any M satisfying Eq. (4.2), then the sequence of operators $W(\alpha F_n)$, $\alpha\in\mathbb{R}$, converges in the weak topology defined by the states $\mathbb{F}$. In fact, in each representation $\Pi_{M,\lambda}$ defined by the states $\omega_{M,\lambda}$, $W(\alpha F_n)$ is a strongly convergent Cauchy sequence as a consequence of (5.1) [the calculation is similar to that of Eq. (A1′) in the Appendix]. Moreover,

$$\begin{aligned}&\lim_{n\to\infty}\omega_{M,\lambda}(W(G_1)W(\alpha F_n)W(G_2))\\ &\quad=e^{i\lambda\alpha}\omega_{M,\lambda}(W(G_1)W(G_2)),\quad\forall G_1,G_2\in\mathscr{F}\,.\end{aligned} \tag{5.2}$$

We can then define

$$U(\alpha)=\text{s-}\lim_{n\to\infty}W(\alpha F_n)\,, \tag{5.3}$$

with the properties

$$U(\alpha)U(\beta) = U(\alpha+\beta)\,, \tag{5.4}$$

$$\Pi_{M,\lambda}(U(\alpha)) = e^{i\lambda\alpha}\,. \tag{5.5}$$

This implies that $U(\alpha)$ is strongly continuous in α and its generator is well defined,

$$U(\alpha) = \exp i\alpha\varphi_\infty\,, \tag{5.6}$$

it commutes with the field algebra $\mathscr{A}$, and

$$\Pi_{M,\lambda}(e^{i\alpha\varphi_\infty}) = e^{i\lambda\alpha}\,. \tag{5.7}$$

The algebraic dynamics α^t can now be characterized in a simple form by using (4.6) and (5.7)

$$\alpha^t(W(F)) = W(F^t)\exp\{i\varphi_\infty[\tilde{f}_1(0)(1-\cos\omega_0 t) - \tilde{f}_2(0)\omega_0^{-1}\sin\omega_0 t]\}\,, \tag{5.8}$$

$\omega_0 \equiv \omega(k=0)$.

The operators $U(\alpha)$, $\alpha\in\mathbf{R}$ generate by linear combination and norm closures an algebra $\mathscr{A}_\infty$ of *variables at infinity*.

The chiral transformations β^λ, originally defined on $\mathscr{A}$ [Eq. (3.10)] can be uniquely extended to an automatically weakly continuous automorphism of $\mathscr{M} = \bar{\mathscr{A}}$ (see Proposition 4.1 of Ref. 8).

In particular, we have

$$\beta^\lambda(\exp i\alpha\varphi_\infty) = \beta^\lambda \lim_n W(\alpha F_n) = \lim_n \beta^\lambda W(\alpha F_n)$$

$$= e^{i\alpha\lambda}\lim_n W(\alpha F_n) = e^{i\alpha(\varphi_\infty+\lambda)}\,. \tag{5.9}$$

Summarizing, we have the following.

Proposition 5.1: The infrared cutoffed dynamics α_L^t converges strongly, as $L\to\infty$, to the dynamics α^t defined by Eq. (5.8). This α^t does not map the quasilocal algebra $\mathscr{A}$ into itself, but rather it maps $\mathscr{A}$ into the algebra $\mathscr{G}(\mathscr{A}\cup\mathscr{A}_\infty)$, generated (through linear combinations and norm closures) by $\mathscr{A}$ and the algebra at infinity $\mathscr{A}_\infty$.

Furthermore, α^t commutes with the chiral transformations β^λ (*chiral symmetry* of the dynamics).

The latter statement follows easily from Eq. (3.10), $F^t\in\mathscr{F}$, and Eq. (5.9).

The above analysis shows that the discussion of the Schwinger model requires a substantial change with respect to the standard Haag–Kastler algebraic framework since the dynamics α^t requires to abandon the quasilocal algebra $\mathscr{A}$ and to introduce infinitely delocalized variables.

In each irreducible representation Π of $\mathscr{A}$, the variables at infinity are represented by c numbers and therefore it is natural to define an "effective dynamics" α_Π^t, with reference to the representation Π obtained by freezing φ_∞ to its expectation value in Π. For example, if Π is the representation defined by a ground state $\omega_{M,\lambda=0}$ invariant under time translations, which is equivalent to

$$M^t = M\,,$$

or to

$$M = \begin{pmatrix}\omega(k)^{-1} & 0\\ 0 & \omega(k)\end{pmatrix} \equiv M_0\,, \tag{5.10}$$

we have

$$\alpha_\Pi^t W(F) = W(F^t)\,. \tag{5.11}$$

More generally, if $\{\omega_{M,\lambda=0}\}$ is a set of states invariant under time translations, the corresponding effective dynamics $\alpha^t_{\{\omega_M\}}$ satisfies Eq. (5.11), and it is rather obvious to extend the definition to the case $\lambda\neq 0$ and to the case of a set of states $\{\omega_{M,\lambda=\bar{\lambda}}\}$ which is stable under $(\alpha^t)^*$.

It also follows from (5.8) that every state $\omega_{M_0,\lambda}$, $\lambda\in\mathbf{R}$, is a ground state for α^t, but only $\omega_{M_0,\lambda}$ is a ground state for α_{Π_λ}. Therefore a pragmatic point of view in which the algebra is $\mathscr{A}$ and the algebraic dynamics is taken to be α_Π^t rules out the possibility of considering different ground states corresponding to different physical situations. In particular, this prevents the discussion of spontaneous symmetry breaking connected to such different ground states.

VI. CLASSICAL MOTION AT INFINITY. DYNAMICAL SYMMETRIES

To discuss chiral symmetry breaking, according to the general framework of Ref. 6, given a representation Π with space-time translationally invariant ground state ω_0, with $M = M_0, \lambda = 0$, it is convenient to consider the set of states S obtained from ω_0 by applying $(\beta^\lambda)^*$ and $(\alpha_\Pi^t)^*$. Since

$$((\alpha_\Pi^t)^*(\beta^\lambda)^*\omega_0)(W(G)) \equiv \omega_0(\beta^\lambda\alpha_\Pi^t(W(G))) = \omega_0(W(G))\exp[i\lambda(\tilde{g}_1(0)\cos\omega_0 t + \tilde{g}_2(0)\omega_0^{-1}\sin\omega_0 t)]\,, \tag{6.1}$$

the set of states S are the states of the form[21]

$$\omega_{\lambda,\mu}(W(G)) = e^{i\lambda\tilde{g}_1(0)}e^{i\mu\tilde{g}_2(0)}\omega_0(W(G))\,. \tag{6.2}$$

By simple computations one gets

$$(\beta^\lambda)^*\omega_{\lambda_1,\mu_1} = \omega_{\lambda_1+\lambda,\mu_1}\,, \tag{6.3}$$

$$(\alpha_\Pi^t)^*\omega_{\lambda,\mu}(W(G)) = e^{i\lambda\tilde{g}_1^t(0)}e^{i\mu\tilde{g}_2^t(0)}\omega_0(W(G)) = \omega_{\lambda',\mu'}(W(G))\,, \tag{6.4}$$

where

$$\lambda' \equiv \lambda\cos\omega_0 t - \mu\omega_0\sin\omega_0 t,\qquad \mu' \equiv \lambda\omega_0^{-1}\sin\omega_0 t + \mu\cos\omega_0 t\,. \tag{6.5}$$

The set of states S allows the construction of another variable at infinity besides φ_∞. As in Sec. V one can prove that, choosing $G_n = (0,g_n)$, $\tilde{g}_n(0) = 1$, $\forall n$,

$$\lim_{n\to\infty}[G_n,G_n]_M = 0\,, \tag{6.6}$$

in each representation defined by the $\omega_{\lambda\mu}$, the sequence $W(\alpha G_n)$ is strongly convergent. As before, one then puts

$$V(\alpha) \equiv \text{s-}\lim_{n\to\infty} W(\alpha G_n) \tag{6.7}$$

(where the strong limit is with respect to the strong topology of the states S) and

$$V(\alpha) \equiv \exp i\alpha\pi_\infty\,, \tag{6.8}$$

with

$$\omega_{\lambda,\mu}(e^{i\alpha\pi_\infty}) = e^{i\alpha\mu}\,. \tag{6.9}$$

Then, with a slight abuse of language, by using Eqs. (6.4), (6.5), (6.8), and (6.9) one has

$$\omega_{\lambda,\mu}(\alpha_\Pi^t(\varphi_\infty)) = \omega_{\lambda',\mu'}(\varphi_\infty) = \lambda' = \omega_{\lambda,\mu}(\varphi_\infty \cos\omega_0 t - \pi_\infty \omega_0 \sin\omega_0 t), \tag{6.10}$$

$$\omega_{\lambda,\mu}(\alpha_\Pi^t(\pi_\infty)) = \omega_{\lambda,\mu}(\varphi_\infty \omega_0^{-1} \sin\omega_0 t + \pi_\infty \cos\omega_0 t), \tag{6.11}$$

i.e., the following motion of the variables at infinity defined with reference to states S:

$$\begin{aligned} \alpha_\Pi^t \varphi_\infty &= \varphi_\infty \cos\omega_0 t - \pi_\infty \omega_0 \sin\omega_0 t, \\ \alpha_\Pi^t \pi_\infty &= \varphi_\infty \omega_0^{-1} \sin\omega_0 t + \pi_\infty \cos\omega_0 t. \end{aligned} \tag{6.12}$$

By Eqs. (6.3) and (6.4) the automorphisms β^λ, $\lambda\in\mathbb{R}$, α_Π^t, $t\in\mathbb{R}$, generate a three-parameter group $\mathcal{G}$ on S, isomorphic to *rotations and translations in the plane (λ,μ) (dynamical symmetry group)*. In particular, $\mathcal{G}$ contains the one-parameter subgroup of translations of the variable μ, which corresponds to the following automorphism:

$$\gamma^\mu(W(F)) = W(F)e^{i\mu\tilde{f}_2(0)}. \tag{6.13}$$

Clearly

$$\gamma^\mu(e^{i\alpha\pi_\infty}) = e^{i\alpha(\pi_\infty+\mu)}. \tag{6.14}$$

VII. SPONTANEOUS BREAKING OF CHIRAL SYMMETRY AND MASS GENERATION

We are now able to give a rigorous discussion of the breaking of chiral symmetry along the lines of a generalized Goldstone theorem[6] and prove that the *generalized Goldstone bosons have a nonzero mass.* (Mass generation associated to chiral symmetry breaking.)

We start by noticing that the chiral symmetry β^λ, Eq. (3.10), as well as the symmetry γ^μ defined by Eq. (6.13), are locally generated by local currents in the sense that there exist local charges Q_R and T_R, respectively, with the property that for any A of the form $A = W(F)$, $F\in\mathcal{F}$,

$$\beta^\lambda(A) = \|\,\| - \lim_{R\to\infty} e^{iQ_R\lambda} A e^{iQ_R\lambda} \equiv \|\,\| - \lim_{R\to\infty} \beta_R^\lambda(A), \tag{7.1}$$

$$\gamma^\mu(A) = \|\,\| - \lim_{R\to\infty} e^{iT_R\mu} A e^{-iT_R\mu} \equiv \|\,\| - \lim_{R\to\infty} \gamma_R^\mu(A) \tag{7.2}$$

and that, uniformly in λ and μ,

$$\frac{d}{d\lambda}\beta^\lambda(A) = \|\,\| - \lim_{R\to\infty} \frac{d}{d\lambda}\beta_R^\lambda(A), \tag{7.3}$$

$$\frac{d}{d\mu}\gamma^\mu(A) = \|\,\| - \lim_{R\to\infty} \frac{d}{d\mu}\gamma_R^\mu(A). \tag{7.4}$$

In fact, letting

$$e^{iQ_R\lambda} \equiv W(G_R), \quad G_R = (0,\lambda f_R), \tag{7.5}$$

with $f_R(x) = f(|x|/R)$, $f(x) = 1$, for $|x|<1$, $f(x) = 0$ for $|x|>1+a$, $f\in\mathcal{D}$, we have

$$\begin{aligned} W(G_R)W(F)W(-G_R) &= W(G_R)W(F-G_R)e^{i\langle F,G_R\rangle/2} \\ &= W(F)\exp\{(i/2)[\langle F,G_R\rangle - \langle G_R,F-G_R\rangle]\} \\ &= W(F)\exp i\langle F,G_R\rangle, \end{aligned}$$

which converges in norm as $R\to\infty$ to

$$W(F)e^{i\lambda\tilde{f}_1(0)} = \beta^\lambda W(F), \tag{7.6}$$

since $\langle F,G_R\rangle \to \lambda\tilde{f}_1(0)$. Similarly one proves Eq. (7.2).

Equation (7.1) implies that the derivative $(d/d\lambda)\beta_R^\lambda(A)$ exists in the norm topology and

$$\frac{d}{d\lambda}\beta_R^\lambda(A) = W(F)e^{i\langle F,G_R\rangle} i\int dx\, f_1(x) f_R(x) \tag{7.7}$$

converges in norm as $R\to\infty$ to $d\beta^\lambda(W(F))/d\lambda$, i.e., Eq. (7.3) holds. Similarly one proves Eq. (7.4).

Since all the above convergences are in the norm topology (and the product is jointly continuous in this norm), the above results extend to the algebra $\mathcal{A}_0$ finitely generated by the Weyl operators $W(F)$, $F\in\mathcal{F}$. Furthermore, in any representation of $\mathbb{F}$ on a suitable dense domain

$$\frac{d}{d\lambda}\beta_R^\lambda(A) = i[Q_R,A], \quad \forall A\in\mathcal{A}_0 \tag{7.8}$$

and therefore (on that domain)

$$\frac{d}{d\lambda}\beta^\lambda(A)\Big|_{\lambda=0} = i\lim_{R\to\infty}[Q_R,A]. \tag{7.9}$$

This shows that one of the crucial (technical) assumptions of the Goldstone theorem is satisfied by the chiral symmetry β^λ (and by γ^μ as well).

The next step is to check that the charge (density) $\pi(x)$ which generates the chiral symmetry is integrable as a commutator [for more details see Sec. 4, Eq. (4.4) of Ref. 6]. In fact, on a suitable dense domain in which Eq. (7.9) holds, we have

$$[\pi(x),W(F)] = W(F)f_1(x),$$

$F = (f_1,f_2)\in\mathcal{F}$, and clearly we have integrability in x. This property obviously extends to the algebra $\mathcal{A}_0$.

Finally, as shown in the previous section, β^λ, $\lambda\in\mathbb{R}$, and α_Π^t, $t\in\mathbb{R}$, generate the three-parameter group $\mathcal{G}$ on S, isomorphic to rotations and translations in the plane (λ,μ) and therefore condition β' of Ref. 6 is satisfied (and therefore also condition β holds). This means that only a finite number of charges $Q_R(t)$, $t\in\mathbb{R}$, associated to the time evolution of the chiral charge, are independent: here one has only two independent charges and one can take $\pi(f_R)$ and $\varphi(f_R)$.

The analogous condition in terms of "classical motion at infinity" also holds as a consequence of Eqs. (6.12), the motion of the variable at infinity φ_∞ associated to the breaking of chiral symmetry involves only another variable at infinity π_∞ and it actually is a periodic motion with frequency ω_0.

We can then apply the generalized Goldstone theorem of Ref. 6, to show that the *spontaneous breaking of chiral symmetry*

$$i\lim_{R\to\infty}\langle[Q_R,\varphi(f)]\rangle_0 = \tilde{f}(0) \neq 0,$$

implies the existence of generalized Goldstone's bosons with nonzero energy $E=m=\sqrt{e^2}$ in the limit $k=0$ (mass gap associated to chiral symmetry breaking). They are, in fact, the elementary excitations of the theory.

VIII. THE CHIRAL SCHWINGER MODEL

A similar discussion can also be done for the chiral Schwinger model described by the following (formal) Hamiltonian in bosonized form:

$$H=\frac{1}{2}\int dx[\pi^2+(\partial_1\varphi)^2] - \frac{e^2}{4}\int dx\,dy(\partial_1\varphi+\pi)(x)|x-y|(\partial_1\varphi+\pi)(y)\,. \tag{8.1}$$

Introducing as in Sec. III an infrared cutoff

$$V(x)=\tfrac{1}{2}|x|\to V_L(x)\equiv\tfrac{1}{2}|x|f_L(x)\,,$$

one gets a regularized dynamics α_L^t with

$$\alpha_L^t\Phi(F)\equiv\alpha_L^t(\varphi(f_1)+\pi(f_2)) = \Phi(F_L^t)=\Phi(e^{K_L t}F)\,, \tag{8.2}$$

$$\tilde{K}_L(k)=\begin{pmatrix}-ik\tilde{V}_L & -k^2(1+\tilde{V}_L)\\ 1+\tilde{V}_L & -ik\tilde{V}_L\end{pmatrix}. \tag{8.3}$$

The existence of a vacuum state ω amounts to the existence of a positive matrix $\tilde{M}(k)$ with $\omega(W(F))=\exp\{-\frac{1}{4}[F,F]_M\}$ (see Sec. II) and the invariance of ω under time translations requires

$$\tilde{K}_L^{\dagger}\tilde{M}=-\tilde{M}\tilde{K}_L\,, \tag{8.4}$$

i.e.,

$$\tilde{M}_{12}=-\tilde{M}_{21},\quad \tilde{M}_{22}=k^2\tilde{M}_{11}\,. \tag{8.5}$$

Furthermore, the condition that M defines a real quadratic form on the real functions $F(x)$ yields that M can be taken Hermitian and actually such that

$$\tilde{M}_{ij}(k)=\overline{\tilde{M}}_{ij}(-k)\,. \tag{8.6}$$

On the other hand, condition (2.18) gives $\tilde{M}_{12}=\tilde{M}_{21}$ and $\tilde{M}_{11}\tilde{M}_{22}-\tilde{M}_{12}^2=1$; therefore, by Eq. (8.5), $\tilde{M}_{12}=0=\tilde{M}_{21}$, and $\tilde{M}_{22}=|k|$.

To obtain the energy spectrum, we start by looking at the eigenvalues of $K_L(k)$

$$\lambda_1=ik,\quad \lambda_2=-ik-2ik\tilde{V}_L(k)\,. \tag{8.7}$$

Thus the field $\partial_1\varphi-\pi$ is massless, whereas the field $\partial_1\varphi+\pi$ has a frequency spectrum given by

$$\omega_L(k)=-k(1+2\tilde{V}_L)\,. \tag{8.8}$$

One can show that the space-time translationally invariant ground state ω defines a representation in which the energy spectrum is positive. Equation (8.7) then implies that in the $\lim L\to\infty$ the energy spectrum of the elementary excitations is given

$$\omega(k)=k,\quad \text{for } k>0\,,$$
$$\omega(k)=\omega_\infty(k)=-(k+e/k),\quad \text{for } k<0\,.$$

This is clearly a pathological spectrum since it is unbounded for $k\to 0$. Furthermore, this spectrum is not compatible with relativistic invariance and with locality.

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APPENDIX: PROOF OF PROPOSITION 4.1

(A) Since $\alpha_L^t\beta^\lambda=\beta^\lambda\alpha_L^t$, the convergence on the states (4.1) is independent of λ and it suffices[22] to consider the case $\lambda=0$. We will denote by Ψ_0^M the ground (Fock) state corresponding to ω_M.

We start by considering the strong convergence of

$$\alpha_L^t(W(F))W(G)\Psi_0^M,\quad \forall F,G\in\mathcal{F}\,. \tag{A1}$$

Since

$$\|[W(F_L^t)-W(F_{L'}^t)]W(G)\Psi_0^M\|^2 = 2(1-\mathrm{Re}\{\exp(-\tfrac{1}{4}[F_L^t-F_{L'}^t,F_L^t-F_{L'}^t]_M + i\langle F_L^t-F_{L'}^t,G\rangle+(i/2)\langle F_L^t,F_{L'}^t\rangle)\})\,, \tag{A1'}$$

this is equivalent to the convergence of F_L^t in the norm $\|\ \|_M$ defined by the positive scalar product $[\cdot,\cdot]_M$, which also dominates the symplectic form [Eq. (2.7)]. Now, we have

$$\|F_L^t-F_{L'}^t\|_M=\int dk\,B_{jm}^{t,L,L'}(k)\bar{\tilde{f}}_j(k)\tilde{f}_m(k)\,, \tag{A2}$$

$$B_{jm}^{t,L,L'}\equiv(A_{L'}^t-A_L^t)_{ji}^t M_{il}(A_{L'}^t-A_L^t)_{lm}\,, \tag{A3}$$

and $B_{jm}^{t,L,L'}(k)\to 0$ pointwisely, as a consequence of $\tilde{V}_L(k)\to\tilde{V}(k)$ [which implies $\omega_L(k)\to\omega(k)$] and therefore by the Lebesgue dominated convergence theorem it is enough to bound B uniformly in L,L', by a locally integrable function of k. In fact, since

$$|\omega_L^{-1}\sin\omega_L t|\leqslant\omega_L^{-1}(\omega_L|t|)=|t|\,, \tag{A4}$$

we have

$$|B_{11}|\leqslant 4[(1+\alpha^2)^{1/2}r^{-1}+(1+\alpha^2)^{1/2}rt^2+2|\alpha|\,|t|]\,, \tag{A4'}$$
$$|B_{22}|\leqslant 4\Big[(1+\alpha^2)^{1/2}r^{-1}(\sup_L\omega_L(k))^2 + (1+\alpha^2)^{1/2}r+2|\alpha|\sup_L(\omega_L(k))\Big]\,,$$

and the rhs's are elements of $L^1{}_{\mathrm{loc}}$ by (2.18) and (4.2). A similar bound for the off diagonal element $B_{12}=B_{21}$ follows from $\det(A_L^t M A_{L'}^t)=1$:

$$B_{12}^2=B_{11}B_{22}-1\leqslant B_{11}B_{22}\,. \tag{A5}$$

Hence

$$\|\ \|_M-\lim_{L\to\infty}F_L^t=F^t\equiv A^t F\in\mathcal{F}\,, \tag{A6}$$

where F^t is ($\|\ \|_M$ equivalent to) a C^∞ function which for $k\neq 0$ is the pointwise limit of $F_L^t(k)$, and

$$A^t=\begin{pmatrix}\cos\omega t & \omega^{-1}\sin\omega t\\ -\omega\sin\omega t & \cos\omega t\end{pmatrix},\quad \omega=\sqrt{k^2+e^2}\,. \tag{A7}$$

Equation (4.10) implies that the vectors (4.5) are strongly convergent.

Furthermore, since the linear span D^M generated by the

vectors of the form $\Sigma_i \lambda_i W(G_i)\Psi_0^M$, with $G_i \in \mathcal{F}$ and Σ a finite sum, is strongly dense in the Fock space $\mathcal{H}^M$ defined by Ψ_0^M, and $\| W(F_L^t) \| = 1$, $\forall L$, one gets the convergence of $W(F_L^t)$ on $\mathcal{H}^M$. Moreover, since the Weyl operators are bounded, one has the strong convergence of the norm limits

$$\operatorname*{norm\text{-}lim}_{N\to\infty} \sum_{i=1}^{N} a_i W(A_L^t F_i)$$

and therefore the strong convergence[23] of α_L^t on the whole algebra $\mathcal{A}$.

(B) To determine the mapping $(\alpha^t)^*$ we consider the $\lim_{L\to\infty} (\alpha_L^t)^*$ on the states ($\equiv D^{M,\lambda}$) of the form

$$\phi_{M,\lambda}^{G_1,G_2}(\mathcal{A}) = \omega_{M,\lambda}(W(G_1)\mathcal{A}W(G_2)),$$
$$G_{1,2} \in \mathcal{F}, \quad \tilde{G}_{1,2}(0) = 0, \tag{A8}$$

and we have [by Eq. (4.10) and $\tilde{f}_{1,L}^t(0) = \tilde{f}_{1,L}(0)$, $\forall L$]

$$\begin{aligned}\lim_{L\to\infty} & \omega_{M,\lambda}(W(G_1)\alpha_L^t(W(F)))W(G_2) \\ &= \exp\{-\tfrac{1}{4}\|G_1 + G_2 + F^t\|_M\}\exp i\lambda\tilde{f}_1(0) \\ &\quad \times\exp\{-(i/2)(\langle G_1,G_2\rangle + \langle G_1,F^t\rangle + \langle F^t,G_2\rangle)\} \\ &= \phi_{M^t,\lambda}^{G_1^{-t},G_2^{-t}}(W(F)), \end{aligned} \tag{A9}$$

where

$$M^t \equiv (A^\dagger)^t M A^t. \tag{A10}$$

One can easily check that if M satisfies conditions (4.2), so does M^t and the state (A9) is a state of the form (A8). In fact, by a bound similar to that used for B [Eqs. (A4), (A4′)] we get

$$|M_{11}(t)| \leqslant M_{11} + M_{22}t^2 + 2|M_{12}|\,|t|,$$
$$|M_{22}(t)| \leqslant M_{11}\omega^2 + M_{22} + 2M_{12}\omega,$$

and since $\omega(k)$ is locally bounded we obtain Eq. (4.2). Since $\det M(t) = \det M$, a similar bound is obtained for $M_{12}(t)$ [see Eq. (A5)]. Thus $(\alpha^t)^*$ maps states of the form (A8) into states of the same form. Furthermore, since $(\alpha^t)^*$ is always continuous in norm and strongly convergent vectors define states which converge in norm, $(\alpha^t)^*$ maps the pure states of $\mathcal{H}^{M,\lambda}$ [norm limit of states defined by linear combination of vectors appearing in Eq. (A8)] into states which are the norm limits of states of the same form in $\mathcal{H}^{M,\lambda}$, i.e., pure states of $\mathcal{H}^{M^t,\lambda}$, $\forall M,\lambda$. In conclusion, Eq. (4.3) holds.

On the states of $D^{M,\lambda}$ [see Eq. (A8)] the group property of $(\alpha^t)^*$ follows from the group property of A^t; since $D^{M,\lambda}$ is dense in $\mathcal{H}^{M,\lambda}$ and $(\alpha^t)^*$ is norm continuous, the property holds on all the states of $\mathcal{H}^{M,\lambda}$, $\forall M,\lambda$.

(C) Property (C) follows from (B) according to Propositions 2.2 and 2.3 of Ref. 6.

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[14] That is, the strong continuity of $W(\lambda F)$ with respect to $\lambda \in \mathbb{C}$.
[15] For example, by considering a Fock representation of $\mathcal{A}$ corresponding to a nonzero mass.
[16] These details will be discussed separately in a more general framework.
[17] Since $\det M = 1$, this also implies $M_{12} \in L^1_{\rm loc}$.
[18] In the following we will often drop the $\hat{}$, since the states $\mathbb{F}$ are uniquely determined by Eq. (4.1).
[19] Clearly, since fields are singular objects (actually distributions), the meaning of $\varphi(\infty)$ is problematic.
[20] A possible choice is $f_{1,n}(x) = f(x/R_n)/R_n$, with $\int f(x)dx = 1$, $R_n = n\bar{R}$; then $\tilde{f}_{1,n}$ converges to zero pointwisely almost everywhere and Eq. (5.1) holds because $M_{ij}(k) \in L^1_{\rm loc}$.
[21] More generally, one can construct the states $S_{\{M\}}$ associated to a family $\{\omega_{M,\bar{\lambda}}\}$ of states, stable under $(\alpha^t)^*$. If M is an arbitrary matrix satisfying (4.2), then the corresponding $S_{\{M\}} \supset \mathbb{F}$ and $(\alpha_\Pi^t)^*$ does not map $\mathbb{F}$ into $\mathbb{F}$, so that α_Π^t is not $\mathbb{F}$-weakly continuous.
[22] This can also be checked explicitly by applying the argument below to $\omega_{M,\lambda}$.
[23] Convergence of F_L^t to $F^t \in \mathcal{F}$ in the norm $\| \|_M$ has nothing to do with the norm convergence of $W(F_L^t)$, which is in fact excluded by the appearance of variables at infinity [see Eq. (5.8)].

Cosmological models in globally geodesic coordinates. I. Metric

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A thought method of measuring distances and recording times by using light signals and the observer's own clock is introduced into cosmological models of homogeneous and isotropic universes. From this a coordinate transformation that brings the Robertson–Walker metric into a new coordinate system is derived. It is found that this system is a globally geodesic coordinate system that reduces to a local inertial frame at the position of the observer who is moving freely with the cosmological fluid.

I. INTRODUCTION

Einstein's principle of equivalence says that in a small region of space-time one cannot in principle distinguish between the action of a gravitational field and an acceleration locally. In other words, a freely falling observer in a gravitational field cannot detect the gravitational field by physical experiments in his immediate neighborhood; for him all events occur as in an inertial system. Mathematically this principle of equivalence can be expressed as follows: Given any point P_0 in a Riemann space-time, there exist coordinate systems in which

$$g_{\mu\nu}(P_0) = \eta_{\mu\nu}\,, \tag{1}$$

$$g_{\mu\nu,\alpha}(P_0) = 0\,, \tag{2}$$

where $\eta_{\mu\nu}$ is the Minkowski metric and $g_{\mu\nu,\alpha} \equiv \partial g_{\mu\nu}/\partial x^{\alpha}$. Such coordinate systems are said to be local inertial frames. The metric $g_{\mu\nu}$ describes the behavior of clocks and sticks in these frames, exactly as in special relativity. In such a system, the usual laws of electrodynamics, mechanics, etc., in the special relativistic form are locally valid.

Local geodesic coordinate systems at P_0 are those in which geodesics of freely falling particles are straight lines. They satisfy the same conditions (1) and (2) and therefore are identified with local inertial frames at P_0.[1,2] In many applications one is interested in the outcome measurements performed by a special observer; then one will link the coordinate system with the observer. Thus the coordinate system naturally has a physical meaning. The local geodesic coordinate system of a freely falling observer at the point in question is the best approximation to the Minkowski world. However, it can only be introduced in the immediate neighborhood of the point, and hence the influence of the space curvature could not be described within that system. For this purpose the natural way for the observer is to extend the coordinate axes of this frame to larger distances along geodesic lines. Thus the observer can set up a global coordinate system that reduces to a local geodesic coordinate system at the point of the space-time, and therefore we can call this system a globally geodesic coordinate system accordingly. In this system the influence of the space curvature can directly be reflected by the deviation of $g_{\mu\nu}$ from the Minkowski metric, and the freely falling observer can establish the action of the gravitational field by examining larger regions of space-time conveniently.

One of the significant fields, for which such systems are appropriate to be used, is the observation of gravitational waves. In that case if, say, an observer on the Earth observes the motion of the moon in the field of gravitational waves, he may find that his own globally geodesic coordinate system is possibly the most suitable frame for him, since he is a freely falling observer and the Earth is a freely falling particle. Some research has been done and some interesting results have been derived.[3,4]

Another field is the cosmological models in which all particles are moving freely. Our galaxy is one of these freely falling particles on which a properly constructed globally geodesic coordinate system is possible and may have a particular significance. The goal of this paper is to set up such a system of a typical galaxy and to study the properties of the metric tensor in the system.

II. CONSTRUCTION OF THE COORDINATES

Most cosmological models are based upon the cosmological principle, i.e., the homogeneity and isotropy of the universe. Such models use a comoving coordinate system $\tilde{S}$ in which the metric tensor takes the Robertson–Walker form,

$$ds^2 = d\tilde{t}^{\,2} - a^2(\tilde{t})\left(\frac{d\tilde{r}^2}{1-k\tilde{r}^2} + \tilde{r}^2\,d\theta^2 + \tilde{r}^2\sin^2\theta\,d\varphi^2\right), \tag{3}$$

where $a(\tilde{t})$ is the expansion factor of the universe, k is the constant curvature of the space, the coordinate time $\tilde{t}$ is a cosmic time that reduces to the proper time at each typical galaxy, and the space coordinates $(\tilde{r},\theta,\varphi)$ are comoving, that is, the cosmological fluid is always at rest relative to these space coordinates.

Now we need a coordinate transformation that could bring the metric (3) from $\tilde{S}$ into the globally geodesic system S. The usual method, as described in many textbooks,[5] could not provide us with a globally rigorous coordinate transformation. We shall try to find another way.

As a starting point we notice the method used in special relativity by an observer at the origin of a inertial frame, that is, he measures the trajectory of a moving particle by sending and receiving light signals with an assumption on the invariance of the light speed. Such a method may be helpful for us to construct the system S of a freely falling observer in cosmological models. We take the following method, which is, of course, a thought method of cosmological measurement for time and distance of galaxies. Put the origin of the three

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space coordinates on a typical galaxy moving with the cosmological fluid. Assume that an observer O is rested on the origin and he possesses a standard clock from which he can read out his own proper time. He measures the distance to any galaxy by sending and receiving light signals and records times of the events that the signals arrive at and are reflected by galaxies by using his own clock and a constraint that the radial velocity of light be invariant and be equal to the constant light speed as in special relativity.

Now consider the following process. The observer O at the origin sent out a single light signal at time t_1. This signal was reflected by a typical galaxy P and then returned. It arrived at the observer and was received at time t_2. Times t_1 and t_2 are recorded by the observer's clock. The event P may be denoted by $P(\tilde{t},\tilde{r})$ in $\tilde{S}$ and by $P(t,r)$ in S. Then from the assumption for the light speed we have

$$t=\tfrac{1}{2}(t_1+t_2),\quad r=\tfrac{1}{2}(t_2-t_1)\,, \tag{4}$$

where the units are chosen such that $c=1$. The relationship between $(\tilde{t},\tilde{r})$ and (t,r) can be derived by using the line element (3). Since light signals satisfy $ds^2=0$, we get two equations corresponding to the travels of the light signal from O to P and P to O, respectively, as follows:

$$\begin{aligned}\int_0^{\tilde{r}}\frac{dr'}{\sqrt{1-kr'^2}}&=\int_{t_1}^{\tilde{t}}\frac{dt'}{a(t')}\,,\\ \int_0^{\tilde{r}}\frac{dr'}{\sqrt{1-kr'^2}}&=\int_{\tilde{t}}^{t_2}\frac{dt'}{a(t')}\,.\end{aligned} \tag{5}$$

Note that $t_1=\tilde{t}_1$ and $t_2=\tilde{t}_2$, since the two definitions of time in the two systems coincide at the origin.

Define

$$f(\tilde{r})\equiv\int\frac{d\tilde{r}}{\sqrt{1-k\tilde{r}^2}}\,,\quad F(\tilde{t})\equiv\int\frac{d\tilde{t}}{a(\tilde{t})}\,, \tag{6}$$

and let $f(0)=0$, then Eqs. (5) become

$$f(\tilde{r})=F(\tilde{t})-F(t_1),\quad f(\tilde{r})=F(t_2)-F(\tilde{t})\,. \tag{5'}$$

From Eqs. (4), t_1 and t_2 can be expressed through t and r as

$$t_1=t-r,\quad t_2=t+r\,. \tag{4'}$$

Substituting (4') into (5') and solving (5'), we obtain

$$f(\tilde{r})=\tfrac{1}{2}[F(t+r)-F(t-r)]\,, \tag{7}$$

$$F(\tilde{t})=\tfrac{1}{2}[F(t+r)+F(t-r)]\,. \tag{8}$$

If we make partial derivatives of Eqs. (7) and (8) with respect to t and r, respectively, and take the definitions (6) into account, we get a coordinate transformation as follows:

$$\frac{\partial\tilde{t}}{\partial t}=\frac{1}{2}a(\tilde{t})\left[\frac{1}{a(t+r)}+\frac{1}{a(t-r)}\right], \tag{9a}$$

$$\frac{\partial\tilde{t}}{\partial r}=\frac{1}{2}a(\tilde{t})\left[\frac{1}{a(t+r)}-\frac{1}{a(t-r)}\right], \tag{9b}$$

$$\frac{\partial\tilde{r}}{\partial t}=\frac{1}{2}\sqrt{1-k\tilde{r}^2}\left[\frac{1}{a(t+r)}-\frac{1}{a(t-r)}\right], \tag{9c}$$

$$\frac{\partial\tilde{r}}{\partial r}=\frac{1}{2}\sqrt{1-k\tilde{r}^2}\left[\frac{1}{a(t+r)}+\frac{1}{a(t-r)}\right]. \tag{9d}$$

By the transformation law

$$g_{\alpha\beta}=\frac{\partial\tilde{x}^\mu}{\partial x^\alpha}\frac{\partial\tilde{x}^\nu}{\partial x^\beta}\tilde{g}_{\mu\nu}\,,$$

the metric tensor in the new coordinate system is found to be

$$\begin{aligned}ds^2=&[a^2(\tilde{t})/a(t+r)a(t-r)]\,(dt^2-dr^2)\\&-\tilde{r}^2a^2(\tilde{t})\,(d\theta^2+\sin^2\theta\,d\varphi^2)\,.\end{aligned} \tag{10}$$

III. LOCAL PROPERTIES OF THE COORDINATES

In this section we shall study the local properties of the metric (10). To make comparison with conditions (1) and (2) easier, we express (10) into rectangular coordinates as

$$\begin{aligned}ds^2=&\frac{a^2(\tilde{t})}{a(t+r)a(t-r)}\,dt^2-\frac{\tilde{r}^2a^2(\tilde{t})}{r^2}\,dX^2\\&-\left[\frac{a^2(\tilde{t})}{a(t+r)a(t-r)}-\frac{\tilde{r}^2a^2(\tilde{t})}{r^2}\right]\left(\frac{X\cdot dX}{r}\right)^2,\end{aligned} \tag{11}$$

where X is the position three-vector,

$$\begin{aligned}&dX^2=dx^2+dy^2+dz^2,\\&X\cdot dX=x\,dx+y\,dy+z\,dz=r\,dr,\\&r^2=x^2+y^2+z^2\,.\end{aligned} \tag{12}$$

We denote the origin of the frame as P_0, then Eqs. (7), (8), and (6) yield

$$\tilde{r}(P_0)=0,\quad \tilde{t}(P_0)=t\,. \tag{13}$$

These are trivial results because we have set the two origins of the two systems at the same point where the two times $\tilde{t}$ and t reduce to the proper time of the same observer. Then we can show that the metric (11) satisfies the conditions (1) and (2) at the origin P_0 of the frame (see the Appendix). So we arrive at a conclusion that our coordinate system constructed in Sec. II reduces indeed to a local inertial frame at its origin.

Note that the coordinate transformation (9) is not only a local but also a global transformation, and the metric (10) is a rigorous metric, therefore we call the system a globally geodesic coordinate system.

Another property of the metric (10) is also worth mentioning. That is, since for light signals we have $ds=0$, their radial velocity is invariant at any point of the space-time. This is consistent with the method by which the frame is constructed in Sec. II.

IV. CONCLUSION

In this paper we have derived a rigorous metric describing homogeneous and isotropic universes in a globally geodesic coordinate system. The system reduces to a local inertial frame at its origin on which a freely falling observer moving with the fluid is rested. Therefore it is a naturally space-extended system of the observer's local inertial frame. Because the metric is rigorous globally, it may provide us with some interesting knowledge about the global picture of observations of the universe, i.e., about what the expanding universe looks like to a freely falling observer who carries a standard clock and measures the distances of the galaxies with the use of light signals. In another aspect, since the

frame reduces to a local inertial frame at the origin, it may provide us with a background metric in a neighborhood of the origin. This background metric may be the best approximation of the Minkowski metric with a higher-order correction due to the cosmological field.

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APPENDIX: VERIFICATION OF CONDITIONS (1) AND (2)

In this appendix we shall show that the metric (11) of the main text satisfies conditions (1) and (2) of local inertial frames at the origin P_0 of the coordinates, i.e., at the point $r=0$.

From Eqs. (9) we find, with the use of Eqs. (13), that

$$\frac{\partial\tilde{t}}{\partial t}(P_0)=1,\quad \frac{\partial\tilde{t}}{\partial r}(P_0)=0,\qquad \frac{\partial\tilde{r}}{\partial t}(P_0)=0,\quad \frac{\partial\tilde{r}}{\partial r}(P_0)=\frac{1}{a(t)}. \tag{A1}$$

Then, from (13) and (A1), we get

$$\frac{a^2(\tilde{t})}{a(t+r)a(t-r)}(P_0)=1,$$

$$[\tilde{r}a(\tilde{t})/r](P_0)\equiv\lim_{r\to 0}[\tilde{r}a(\tilde{t})/r] \tag{A2}$$

$$=\lim_{r\to 0}\frac{\partial\tilde{r}/\partial r}{(\partial/\partial r)(r/a(\tilde{t}))}=1.$$

Substituting (A2) into the metric (11), we see that condition (1) is satisfied.

The verification of condition (2) is rather complicated. From the metric (11) we can see that in order to verify condition (2) we need to calculate partial derivatives of two expressions

$$\frac{a^2(\tilde{t})}{a(t+r)a(t-r)}\quad\text{and}\quad\frac{\tilde{r}a(\tilde{t})}{r} \tag{A3}$$

at P_0 with respect to t and x^i $(i=1,2,3)$, respectively. We shall show that all these partial derivatives are equal to zero at the point $r=0$ (or tend to zero as $r\to 0$). First we find

$$\frac{\partial}{\partial t}\left[\frac{a^2(\tilde{t})}{a(t+r)a(t-r)}\right](P_0)$$
$$=\frac{a^2(\tilde{t})}{a(t+r)a(t-r)}\left[2\frac{\dot{a}(\tilde{t})}{a(\tilde{t})}\frac{\partial\tilde{t}}{\partial t}-\frac{\dot{a}(t+r)}{a(t+r)}-\frac{\dot{a}(t-r)}{a(t-r)}\right](P_0)$$
$$=0, \tag{A4}$$

where we have used Eqs. (13) and (A1). From (13) and (A1) we also find

$$\frac{\partial}{\partial r}\left[\frac{a^2(\tilde{t})}{a(t+r)a(t-r)}\right](P_0)$$
$$=\frac{a^2(\tilde{t})}{a(t+r)a(t-r)}\left[2\frac{\dot{a}(\tilde{t})}{a(\tilde{t})}\frac{\partial\tilde{t}}{\partial r}-\frac{\dot{a}(t+r)}{a(t+r)}+\frac{\dot{a}(t-r)}{a(t-r)}\right](P_0)$$
$$=0. \tag{A5}$$

Therefore we have

$$\frac{\partial}{\partial x^i}\left[\frac{a^2(\tilde{t})}{a(t+r)a(t-r)}\right](P_0)$$
$$=\frac{\partial r}{\partial x^i}\frac{\partial}{\partial r}\left[\frac{a^2(\tilde{t})}{a(t+r)a(t-r)}\right](P_0)$$
$$=0, \tag{A6}$$

where i takes the values 1, 2, 3 only.

Now we proceed to deal with the second term of (A3). From (9c) and (9d) we find that

$$\frac{\partial^2\tilde{r}}{\partial r\,\partial t}(P_0)=\left\{-\frac{1}{2}\frac{k\tilde{r}}{\sqrt{1-k\tilde{r}^2}}\left[\frac{1}{a(t+r)}-\frac{1}{a(t-r)}\right]\frac{\partial\tilde{r}}{\partial r}+\frac{1}{2}\sqrt{1-k\tilde{r}^2}\left[-\frac{\dot{a}(t+r)}{a^2(t+r)}-\frac{\dot{a}(t-r)}{a^2(t-r)}\right]\right\}(P_0)$$
$$=-\dot{a}(t)/a^2(t), \tag{A7}$$

$$\frac{\partial^2\tilde{r}}{\partial r^2}(P_0)=\left\{-\frac{1}{2}\frac{k\tilde{r}}{\sqrt{1-k\tilde{r}^2}}\left[\frac{1}{a(t+r)}+\frac{1}{a(t-r)}\right]\frac{\partial\tilde{r}}{\partial r}+\frac{1}{2}\sqrt{1-k\tilde{r}^2}\left[-\frac{\dot{a}(t+r)}{a^2(t+r)}+\frac{\dot{a}(t-r)}{a^2(t-r)}\right]\right\}(P_0)$$
$$=0. \tag{A8}$$

We then find, by using (A1), (A7), and (A8), that

$$\frac{\tilde{r}}{r}(P_0)\equiv\lim_{r\to 0}\frac{\tilde{r}}{r}=\lim_{r\to 0}\frac{\partial\tilde{r}}{\partial r}=\frac{1}{a(t)}, \tag{A9}$$

$$\frac{\partial}{\partial t}\left(\frac{\tilde{r}}{r}\right)(P_0)\equiv\lim_{r\to 0}\frac{\partial}{\partial t}\left(\frac{\tilde{r}}{r}\right)=\lim_{r\to 0}\frac{\partial}{\partial r}\left(\frac{\partial\tilde{r}}{\partial t}\right)=-\frac{\dot{a}(t)}{a^2(t)}, \tag{A10}$$

$$\frac{\partial}{\partial r}\left(\frac{\tilde{r}}{r}\right)(P_0)\equiv\lim_{r\to 0}\frac{\partial}{\partial r}\left(\frac{\tilde{r}}{r}\right)=\lim_{r\to 0}\frac{1}{r}\left(\frac{\partial\tilde{r}}{\partial r}-\frac{\tilde{r}}{r}\right)$$
$$=\lim_{r\to 0}\frac{\partial}{\partial r}\left(\frac{\partial\tilde{r}}{\partial r}-\frac{\tilde{r}}{r}\right)=\lim_{r\to 0}\frac{\partial^2\tilde{r}}{\partial r^2}-\lim_{r\to 0}\frac{\partial}{\partial r}\frac{\tilde{r}}{r}$$
$$=-\lim_{r\to 0}\frac{\partial}{\partial r}\frac{\tilde{r}}{r},$$

therefore

$$\frac{\partial}{\partial r}\left(\frac{\tilde{r}}{r}\right)(P_0)=0. \tag{A11}$$

Now we find

$$\frac{\partial}{\partial t}\left[\frac{\tilde{r}a(\tilde{t})}{r}\right](P_0)\equiv\lim_{r\to 0}\frac{\partial}{\partial t}\left[\frac{\tilde{r}a(\tilde{t})}{r}\right]$$
$$=\lim_{r\to 0}\left[\frac{\tilde{r}\dot{a}(\tilde{t})}{r}\frac{\partial\tilde{t}}{\partial t}+a(\tilde{t})\frac{\partial}{\partial t}\left(\frac{\tilde{r}}{r}\right)\right]$$

$$= \dot{a}(t)\lim_{r\to 0}\frac{\tilde{r}}{r} + a(t)\lim_{r\to 0}\frac{\partial}{\partial t}\left(\frac{\tilde{r}}{r}\right)$$
$$= \frac{\dot{a}(t)}{a(t)} - \frac{\dot{a}(t)}{a(t)}$$
$$= 0\,, \tag{A12}$$

where we have used Eqs. (13), (A1), (A9), and (A10); and

$$\frac{\partial}{\partial r}\left[\frac{\tilde{r}a(\tilde{t})}{r}\right](P_0) \equiv \lim_{r\to 0}\frac{\partial}{\partial r}\left[\frac{\tilde{r}a(\tilde{t})}{r}\right]$$
$$= \lim_{r\to 0}\left[\frac{\tilde{r}\dot{a}(\tilde{t})}{r}\frac{\partial\tilde{t}}{\partial r} + a(\tilde{t})\frac{\partial}{\partial r}\left(\frac{\tilde{r}}{r}\right)\right]$$
$$= \lim_{r\to 0}\left[\frac{\tilde{r}\dot{a}(\tilde{t})}{r}\frac{\partial\tilde{t}}{\partial r}\right] + a(t)\lim_{r\to 0}\frac{\partial}{\partial r}\left(\frac{\tilde{r}}{r}\right)$$
$$= 0\,, \tag{A13}$$

where we have used (13), (A1), (A9), and (A11). Thus from (A13) we find

$$\frac{\partial}{\partial x^i}\left[\frac{\tilde{r}a(\tilde{t})}{r}\right](P_0) = \frac{\partial r}{\partial x^i}\frac{\partial}{\partial r}\left[\frac{\tilde{r}a(\tilde{t})}{r}\right](P_0)$$
$$\equiv \lim_{r\to 0}\frac{\partial r}{\partial x^i}\frac{\partial}{\partial r}\left[\frac{\tilde{r}a(\tilde{t})}{r}\right]$$
$$= 0\,, \tag{A14}$$

where $i = 1,2,3$. Then we see, from (A4), (A6), (A12), and (A14), that the metric (11) also satisfies condition (2).

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[2] H. Stephani, *General Relativity* (Cambridge U.P., Cambridge, 1982), pp. 20 and 66.

[3] L. P. Grishchuk and A. G. Polnarev, in *General Relativity and Gravitation*, edited by A. Held (Plenum, New York, 1980), Vol. 2, p. 393.

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[5] See, for example, C. W. Misner, K. S. Thorne, and J. A. Wheeler, *Gravitation* (Freeman, San Francisco, 1973), p. 285.

Cosmological models in globally geodesic coordinates. II. Near-field approximation

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A near-field approximation dealing with the cosmological field near a typical freely falling observer is developed within the framework established in the preceding paper [J. Math. Phys. **28**, 1920 (1987)]. It is found that for the matter-dominated era the standard cosmological model of general relativity contains the Newtonian cosmological model, proposed by Zel'dovich, as its near-field approximation in the observer's globally geodesic coordinate system.

I. INTRODUCTION

In the preceding paper[1] we have derived a coordinate transformation as

$$f(\tilde{r}) = \tfrac{1}{2}[F(t+r) - F(t-r)]\,, \tag{1}$$

$$F(\tilde{t}) = \tfrac{1}{2}[F(t+r) + F(t-r)]\,, \tag{2}$$

where f and F are defined as

$$f(\tilde{r}) \equiv \int \frac{d\tilde{r}}{\sqrt{1-k\tilde{r}^2}}\,, \tag{3a}$$

$$F(\tilde{t}) \equiv \int \frac{d\tilde{t}}{a(\tilde{t})}\,. \tag{3b}$$

This transformation transforms the Robertson–Walker metric

$$ds^2 = d\tilde{t}^{\,2} - a^2(\tilde{t})\left[\frac{d\tilde{r}^2}{1-k\tilde{r}^2} + \tilde{r}^2\,d\theta^2 + \tilde{r}^2\sin^2\theta\,d\varphi^2\right] \tag{4}$$

of the homogeneous and isotropic universe from a comoving coordinate system into a globally geodesic coordinate system of a freely falling observer with the form

$$ds^2 = \frac{a^2(\tilde{t})}{a(t+r)a(t-r)}(dt^2 - dr^2) - \tilde{r}^2a^2(\tilde{t})(d\theta^2 + \sin^2\theta\,d\varphi^2)\,. \tag{5}$$

For a given point P in the cosmological field, all $\tilde{t}$, $\tilde{r}$, t, and r have definite interpretations: $\tilde{t}$ is the proper time of P; $\tilde{r}$ is the comoving radius, or comoving distance, of P to the origin; t and r are the measured time and distance of the point P by the observer at the origin who uses a standard clock and a constraint on the invariance of the radial speed of light; and $\tilde{t}$ and t coincide and both reduce to observer's proper time at the origin $r = 0$.

The metric (5) reduces to a local inertial frame at the origin of the system.[1] Therefore in a neighborhood of the origin the metric (5) must deviate only slightly from that of a flat space-time, i.e., the gravitational field near the freely falling observer at the origin is weak. So a weak field approximation of a local universe can be developed.

It is well known that the correspondence principle is a fundamental principle in physics. This principle says that a newer, more accurate theory must contain the predecessor as one of its limiting cases. The general relativity has a particularly rich correspondence structure.[2] That is, it has as distinct limiting cases (a) special relativity; (b) the linearized theory of gravity; (c) Newton's theory of gravity; and (d) the post-Newtonian theory of gravity. We shall see in this paper that all of these limits can be arrived at by developing a near-field approximation in a region near the origin of the globally geodesic system.

There are mainly two reasons to believe that the local properties of the universe are described by Newtonian theory. One is based on Birkhoff's theorem[3]; another is based on the correspondence principle between general relativity and Newton's theory.[4–6] The first Newtonian treatment of a static cosmological fluid was given by Jeans in 1902.[7] His work proved to be of utmost importance in the problem of the formation of galaxies, but such a static background does not describe the actual situation in our Universe. The possibility of describing an expanding universe by Newtonian theory is carefully studied by Zel'dovich.[6] He obtained a set of equations that corresponds to the idea of a homogeneous and isotropic universe. We shall show in Sec. V that Zel'dovich's model of an expanding universe is contained in the standard cosmological model of general relativity as a limiting case, and therefore can be regarded as its Newtonian approximation in the globally geodesic coordinate system.

II. NEAR-FIELD APPROXIMATION

We define "near-field" as a space region around the origin of the coordinates of (5), provided that in this region the condition

$$r \ll t \tag{6}$$

is satisfied everywhere. We know that t is the proper time of the observer and therefore the "age" of the universe. This "age" has the same order of magnitude as the space scale of the whole universe. Then we see that the condition (6) holds if the space region considered by the observer is much smaller than the space scale of the whole universe.

We can choose the units to make $t \sim 1$, and then condition (6) means that r is a small parameter and we can expand all required quantities into a power series of the small parameter r.

We shall not follow the normal procedure of weak field approximation in this section. Taking account of the particularity of the problem, we shall adopt a new technique to

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obtain directly the power-series expansions of the coordinate transformation (1) and (2), the expansion factor $a(\tilde{t})$, and the metric tensor (5).

Let us first consider the coordinate transformation (1) and (2). All functions appearing in these equations can be expanded in a Taylor series as follows:

$$F(\tilde{t}) = F(t) + \dot{F}(t)(\tilde{t}-t) + \tfrac{1}{2}\ddot{F}(t)(\tilde{t}-t)^2 + \tfrac{1}{6}\dddot{F}(t)(\tilde{t}-t)^3 + \cdots, \tag{7}$$

$$F(t+r) = F(t) + \dot{F}(t)r + \tfrac{1}{2}\ddot{F}(t)r^2 + \tfrac{1}{6}\dddot{F}(t)r^3 + \tfrac{1}{24}\ddddot{F}(t)r^4 + \cdots, \tag{8}$$

$$F(t-r) = F(t) - \dot{F}(t)r + \tfrac{1}{2}\ddot{F}(t)r^2 - \tfrac{1}{6}\dddot{F}(t)r^3 + \tfrac{1}{24}\ddddot{F}(t)r^4 - \cdots, \tag{9}$$

where $\dot{F}(t) \equiv (d/dt)F(t)$, etc., $f(r)$ can be expanded, by using (3a), as

$$f(\tilde{r}) = \int \frac{d\tilde{r}}{\sqrt{1-k\tilde{r}^2}} = \int \left(1 + \frac{1}{2}k\tilde{r}^2 + \cdots\right)d\tilde{r} = \tilde{r} + \tfrac{1}{6}k\tilde{r}^3 + \cdots. \tag{10}$$

To make Eqs. (7) and (10) power series of r, we assume $\tilde{t}$ and $\tilde{r}$ to be of the form

$$\tilde{t} = t + b_1 r + b_2 r^2 + b_3 r^3 + \cdots, \tag{11}$$

$$\tilde{r} = c_1 r + c_2 r^2 + c_3 r^3 + c_4 r^4 + \cdots. \tag{12}$$

Put (11) and (12) into (7) and (10), respectively, we find

$$F(\tilde{t}) = F(t) + b_1\dot{F}(t)r + [b_2\dot{F}(t) + \tfrac{1}{2}(b_1)^2\ddot{F}(t)]r^2 + [b_3\dot{F}(t) + b_1 b_2\ddot{F}(t) + \tfrac{1}{6}(b_1)^3\dddot{F}(t)]r^3 + \cdots, \tag{13}$$

$$f(\tilde{r}) = c_1 r + c_2 r^2 + [c_3 + \tfrac{1}{6}k(c_1^3)]r^3 + [c_4 + \tfrac{1}{2}k(c_1)^2 c_2]r^4 + \cdots. \tag{14}$$

Substituting Eqs. (8), (9), (13), and (14) into Eqs. (1) and (2), respectively, and equating the coefficients of r^n on both sides of these equations, gives

$$b_1 = 0, \quad b_2 = \ddot{F}(t)/2\dot{F}(t), \quad b_3 = 0, \quad \ldots,$$
$$c_1 = \dot{F}(t), \quad c_2 = 0, \quad c_3 = \tfrac{1}{6}\ddot{F}(t) - \tfrac{1}{6}k\dot{F}^3(t), \quad c_4 = 0, \ldots. \tag{15}$$

From (3b) we can see that

$$\dot{F}(t) = \frac{1}{a(t)}, \quad \ddot{F}(t) = -\frac{\dot{a}(t)}{a^2(t)}, \quad \dddot{F}(t) = -\frac{a(t)\ddot{a}(t) - 2\dot{a}^2(t)}{a^3(t)}. \tag{16}$$

Thus we find, from (11), (12), (15), and (16), the required expansions of $\tilde{t}$ and $\tilde{r}$ of the form

$$\tilde{t} = t - \frac{1}{2}\frac{\dot{a}(t)}{a(t)}r^2 + O(r^4), \tag{17}$$

$$\tilde{r} = \frac{1}{a(t)}r - \frac{a(t)\ddot{a}(t) - 2\dot{a}^2(t) + k}{6a^3(t)}r^3 + O(r^5), \tag{18}$$

where $O(r^n)$ represents terms of order r^n.

The Taylor series of the expansion factor $a(\tilde{t})$ is

$$a(\tilde{t}) = a(t) + \dot{a}(t)(\tilde{t}-t) + \tfrac{1}{2}\ddot{a}(t)(\tilde{t}-t)^2 + \cdots. \tag{19}$$

On applying (17), we obtain

$$a(\tilde{t}) = a(t)\left[1 - \frac{1}{2}\frac{\dot{a}^2(t)}{a^2(t)}r^2 + O(r^4)\right]. \tag{20}$$

To obtain the required expansion of the metric (5), we need also to expand $a(t+r)$ and $a(t-r)$ into Taylor series:

$$a(t+r) = a(t)\left[1 + \frac{\dot{a}(t)}{a(t)}r + \frac{1}{2}\frac{\ddot{a}(t)}{a(t)}r^2 + \frac{1}{6}\frac{\dddot{a}(t)}{a(t)}r^3 + O(r^4)\right], \tag{21}$$

$$a(t-r) = a(t)\left[1 - \frac{\dot{a}(t)}{a(t)}r + \frac{1}{2}\frac{\ddot{a}(t)}{a(t)}r^2 - \frac{1}{6}\frac{\dddot{a}(t)}{a(t)}r^3 + O(r^4)\right]. \tag{22}$$

If we put (20)–(22) and (18) into (5), we get a series expansion of the metric tensor (5) as follows:

$$g_{00} = -g_{11} = \frac{a^2(\tilde{t})}{a(t+r)a(t-r)} = 1 - \frac{\ddot{a}(t)}{a(t)}r^2 + O(r^4),$$
$$g_{22} = (1/\sin^2\theta)g_{33} = -\tilde{r}^2 a^2(\tilde{t}) = -r^2\left[1 - \frac{1}{3}\frac{a(t)\ddot{a}(t) + \dot{a}^2(t) + k}{a^2(t)}r^2 + O(r^4)\right]. \tag{23}$$

Here we make a few remarks about Eqs. (17) and (18), which provide us with not only a coordinate transformation, but, remembering the physical interpretations of $\tilde{t}$ and $\tilde{r}$, these two equations in fact also provide us with a full description of the trajectory of any comoving particles near the origin observed in the globally geodesic coordinate system. Now let us consider another case in which a test particle moves arbitrarily in the field. This particle need not be a comoving particle; its motion may deviate from the background fluid, and therefore $\tilde{t}$ and $\tilde{r}$ may lose their special interpretations as the proper times and the comoving radius of the considered object. In this case we must regard (17) and (18) as only a coordinate transformation, and regard (23) as a background metric where $a(t)$ satisfies Einstein's field equations (see Sec. IV). The trajectory of this test particle is determined naturally by the geodesic equations and approximates to a straight line near the origin.

III. EQUATIONS OF MOTION OF PERFECT FLUID

In this section we shall study the near-field approximation of equations of hydrodynamics for the cosmological perfect fluid.

The energy-momentum tensor of a perfect fluid takes the form

$$T^{\mu\nu} = (\rho + p)u^\mu u^\nu - p g^{\mu\nu}, \tag{24}$$

where u^μ, ρ, and p are the four-velocity, mass density, and pressure of the fluid, respectively. The conservation of the energy-momentum (24) gives the well-known equations of motion of the perfect fluid as[8]

$$[(\rho + p)u^\nu]_{;\nu} = p_{,\nu}u^\nu, \tag{25}$$

$$(\rho + p)u^\mu{}_{;\nu}u^\nu = p_{,\nu}(g^{\mu\nu} - u^\mu u^\nu). \tag{26}$$

In order to find the orders of all the quantities appearing in these two equations, we consider first the order of the four-velocity. In the comoving system it has the components $\tilde{u}_0 = 1, u_i = 0$ $(i = 1,2,3)$. From the transformation law

$$u_\alpha = \frac{\partial \tilde{x}^\mu}{\partial x^\alpha} \tilde{u}_\mu$$

and by using (17), we obtain its components in the globally geodesic coordinate system of (5) as

$$u_0 = \frac{\partial \tilde{t}}{\partial t} = 1 - \frac{1}{2} \frac{a(t)\ddot{a}(t) - \dot{a}^2(t)}{a^2(t)} r^2 + O(r^4) ,$$

$$u_1 = \frac{\partial \tilde{t}}{\partial r} = -\frac{\dot{a}(t)}{a(t)} r + O(r^3) .$$

Then, from (23), we find

$$u^0 = g^{00} u_0 = 1 + \frac{1}{2} \frac{a(t)\ddot{a}(t) + \dot{a}^2(t)}{a^2(t)} r^2 + O(r^4) ,$$

$$u^1 = g^{11} u_1 = [\dot{a}(t)/a(t)]r + O(r^3) . \tag{27}$$

From (17) we find

$$\rho = \rho(\tilde{t}) = \rho(t) + O(r^2) ,$$

$$p = p(\tilde{t}) = p(t) + O(r^2) . \tag{28}$$

Assume ρ and p to be quantities of same order, i.e., of zero-order of r, then we can summarize, from (27) and (28), that

$$\begin{aligned} &\text{quantities of order } r^0\text{: } \rho,\ p,\ \rho_{,0},\ p_{,0},\ u^0,\ u^i_{,j} , \\ &\text{quantities of order } r^1\text{: } \rho_{,i},\ p_{,i},\ u^i,\ u^0_{,i},\ u^i_{,0} , \\ &\text{quantities of order } r^2\text{: } u^0_{,0} , \end{aligned} \tag{29}$$

where i and j take the values of 1, 2, 3 only. The orders of $g_{\mu\nu}$ and their partial derivatives can be directly found from (23).

If we make an approximation of Eq. (25) up to the zero order of r, we get an equation that can be rewritten in a more familiar form

$$\frac{\partial \rho}{\partial t} + \nabla\cdot[(\rho + p)\mathbf{V}] + O(r^2) = 0 , \tag{30}$$

where $\mathbf{V}$ is the usual three-velocity of the fluid. Up to the first order of r, Eq. (26) (for $\mu = i$) reduces to

$$\frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V}\cdot\nabla)\mathbf{V} + O(r^3) = -\frac{1}{2}\nabla g_{00} - \frac{1}{\rho + p}\left(\nabla p + \mathbf{V}\frac{\partial p}{\partial t}\right) . \tag{31}$$

Equations (30) and (31) constitute the equations of motion of the nearby cosmological fluid in globally geodesic coordinate systems with a background metric (23) and with accuracies in fact to first and second orders of r, respectively.

IV. FIELD EQUATIONS OF GRAVITATION

The gravitational field equations are dependent upon the variety of cosmological models theories of gravity. In this section we consider only the standard cosmological model of general relativity known as the Robertson–Walker–Friedmann universe with metric tensor (4) and field equations[3]

$$\dot{a}^2(\tilde{t}) + k = \tfrac{8}{3}\pi G \rho(\tilde{t}) a^2(\tilde{t}) , \tag{32}$$

$$\dot{\rho}(\tilde{t}) + 3[\dot{a}(\tilde{t})/a(\tilde{t})][\rho(\tilde{t}) + p(\tilde{t})] = 0 , \tag{33}$$

where $\dot{a}(\tilde{t}) = (d/d\tilde{t})a(\tilde{t})$, $\dot{\rho}(\tilde{t}) = (d/d\tilde{t})\rho(\tilde{t})$. The version of these two equations in globally geodesic coordinate systems can be obtained simply by changing the variable $\tilde{t}$ to t. Thus we find

$$\dot{a}^2(t) + k = \tfrac{8}{3}\pi G \rho(t) a^2(t) , \tag{34}$$

$$\dot{\rho}(t) + 3[\dot{a}(t)/a(t)][\rho(t) + p(t)] = 0 , \tag{35}$$

which are the gravitational field equations governing the expansion of the universe in globally geodesic systems.

Note that Eqs. (34) and (35) are not approximate but rigorous equations, and that we should not generally identify $\rho(t)$ with $\rho(\tilde{t})$ and $p(t)$ with $p(\tilde{t})$. In fact $\rho(\tilde{t})$ can be expanded, for the matter-dominated era ($p = 0$), as

$$\rho(\tilde{t}) = \rho_0 a_0^3 a^{-3}(\tilde{t}) = \rho(t)\left[1 + \frac{3}{2}\frac{\dot{a}^2(t)}{a^2(t)} r^2 + O(r^4)\right] , \tag{36}$$

where we have used the expansion of $a(\tilde{t})$ in (20).

V. CORRESPONDENCE WITH NEWTONIAN COSMOLOGY

For the matter-dominated era the pressure p is negligible compared with the mass density ρ. Suppose p is of order r^2, then ∇p is of order r^1 and $\partial p/\partial t$ is of order r^2. The equations of motion of the cosmological fluid, (30) and (31), are thus reduced to

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{V}) + O(r^2) = 0 , \tag{37}$$

$$\frac{\partial \mathbf{V}}{\partial t} + (\mathbf{V}\cdot\nabla)\mathbf{V} + O(r^3) = -\frac{1}{2}\nabla g_{00} - \frac{1}{\rho}\nabla p . \tag{38}$$

To the lowest order of r, (37) and (38) are just the same equations in the Newtonian cosmology used by Jeans[7] and Zel'dovich,[6] provided that

$$g_{00} = 1 + 2\varphi , \tag{39}$$

where φ is the Newtonian potential. From (39) and (23) we find

$$\varphi = -\tfrac{1}{2}[\ddot{a}(t)/a(t)]r^2 + O(r^4) . \tag{40}$$

Equations (37)–(40), together with the gravitational field equations of the model, constitute a complete set of equations describing the local behavior of the universe in the observer's geodesic coordinate system.

From (40) we see that the Newtonian potential φ may take different forms of expression through $a(t)$, which is dependent upon the theories of gravity and the models of the universe. The standard cosmological model of general relativity provides us, for the matter-dominated era, with[3]

$$\ddot{a}(t) = -\tfrac{4}{3}\pi G \rho a(t) , \tag{41}$$

so that φ in (40) takes the form

$$\varphi = \tfrac{2}{3}\pi G \rho r^2 + O(r^4) . \tag{42}$$

From (27) we see that the three-velocity $\mathbf{V}$ may be written as

$$\mathbf{V} \equiv [\dot{a}(t)/a(t)]\mathbf{r} = H\mathbf{r} , \tag{43}$$

where

$$H \equiv \dot{a}(t)/a(t) . \tag{44}$$

Then a set of solutions that are the same as those obtained by

Zel'dovich[6] is derived from the standard Robertson–Walker–Friedmann model of general relativity as a limiting case. Thus we arrive at an opinion that Zel'dovich's model of cosmology, which is based on the Newtonian theory, can be regarded as the Newtonian approximation of the standard Robertson–Walker–Friedmann model in the globally geodesic coordinate system with correspondences $g_{00} = 1 + 2\varphi$ and $H = \dot{a}(t)/a(t)$. On this account the Newtonian equations used by Jeans and Zel'dovich are local equations that cannot describe the large scale structure of the universe. Astronomical observations reveal that galaxies and clusters of galaxies are of size $\sim 10^6$ light years and $\sim 10^7$ light years, respectively, and the universe is of age $\sim 10^{10}$ years. Therefore one can use these equations in the problem of the formation of galaxies by keeping in mind that some higher-order terms may appear. The order of such a term may be found from (37), (38), and (40) with $r \sim 10^{-4}$ to 10^{-3} in the present time.

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On Geroch's limit of space-times and its relation to a new topology in the space of Lie groups

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In the space G_n of n-dimensional Lie algebras a new non-Hausdorff topology τ is defined. Here (G_n, τ) is a compact connected T_0 space. The closed one-point sets in the noncommutative part of G_n are called atoms. For each $n \geqslant 3$ there exist two atoms. Geroch's limit defines a topology σ in the space N_n of local homogeneous Riemannian manifolds of dimension n. A natural relation of the N_n to the spaces G_n is given by the Lie algebra corresponding to the isometry group of the elements of N_n. It has nice σ–τ-continuity properties, e.g., the atoms are exactly those elements of G_n that correspond to closed nonempty subsets in the nonflat part of N_n. Applying to cosmology, especially for cosmological models with intrinsically homogeneous slices $t = \text{const}$, a complete answer to the question of how the isometry group of the spacelike hypersurfaces may depend on time is given: The slices are σ-continuous and their isometry groups are τ-continuous functions of time t. Applications of σ and τ to other problems are sketched.

I. INTRODUCTION

A homogeneous cosmological model is a space-time possessing an isometry group acting on spacelike hypersurfaces $V_3(t) \in N_3$, N_3 being the space of local homogeneous three-dimensional Riemannian spaces of signature $+ + +$. As one knows,[1] N_3 can be classified according to the respective Lie groups of isometry of its elements: Bianchi types I,...,IX; VI and VII are one-parameter sets of Lie groups. Additionally, we have the models of Kantowski–Sachs type.[2,3] Each of these types represents a family of cosmological models. But nowadays one does not restrict automatically to one Bianchi type but allows cosmological models whose Bianchi type changes with time. They are called intrinsically homogeneous cosmological models[4,5] for they require only the first (and not the second, too, as one usually does) fundamental form of the slices to be homogeneous.

In Sec. IV we shall show the following: The set N_3 endowed with a topology defined by Geroch's limit is a three-dimensional manifold with boundary and the four invariants

$$R,\ R_{ij}R^{ij},\ R_{ij}R^{jk}R^{i}{}_{k},\ \text{and}\ R_{i[j;k}R^{i[j;k]}$$

give a unique[6] and homeomorphic parametrization of it. (The first three invariants do not suffice!) Further we answer the question of how the Bianchi type can change with time.

To derive these results we introduce a topology τ in the space of Lie groups and give some properties of it in Sec. II; and we consider the topology σ induced by Geroch's limit[7,8] in Sec. III. A comparison of σ and τ is performed in Sec. IV. In the final Sec. V we discuss some possible applications of the topologies σ and τ. In the Appendix we give some basic definitions and results concerning non-Hausdorff topologies to make the paper readable also for those readers who are not familiar with this topic.

In all the derivations we pay essential attention to the underlying topological structures as compactness and separation axioms and what consequences they have.

II. A TOPOLOGY IN THE SPACES OF LIE GROUPS

We shall restrict ourselves to finite-dimensional Lie groups, the infinite-dimensional ones can be thought to be constructed from the finite-dimensional ones by the direct limit with the natural embedding of the set G_n^* of n-dimensional Lie groups into G_{n+1}^* given by the direct product with the real line. Further, the topology to be constructed shall not distinguish between locally isomorphic Lie groups, i.e., the topology will not be T_0 (cf. the Appendix), but its associated T_0 space is homeomorphic to a T_0 topology τ in the space G_n of n-dimensional Lie algebras, and the latter is the object of our study. We take $n \geqslant 2$, for $n = 1$ is trivial.

A. Motivation

Before writing the definition we give some motivations for it. First, consider the surface of a Euclidean sphere of radius r and then the limit $r \to \infty$. Obviously, but also strongly using Geroch's limit (see below), this sequence converges to the Euclidean plane. But what about the Lie groups of isometry? For all spheres it is the same one (Bianchi type IX) but another one (Bianchi type VII_0) for the plane.[3] But we wish to have this limit being valid on the Lie group level, too: $\text{IX} \to \text{VII}_0$ denotes the fact that a sequence of Lie groups all of which are type IX converges to type VII_0, i.e., we do not wish τ to be a T_1 space. It is not desirable at all to make τ a Hausdorff topology, because for $n = 3$ only the two one-parameter sets VI_h and VII_h would give rise to deviations from the discrete topology.

On the other hand, we wish τ to be naturally induced and not prescribed from outside. Therefore, we proceed as follows.

B. Definition of τ

Let R^n be the n-dimensional oriented real vector space and $(e_1,...,e_n)$ a basis of it. As one knows, a Lie product $[e,f]$ in R^n is defined by the structure constants $C^i{}_{jk}$ via the equations

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$$[e_i,e_j] = C^k{}_{ij} e_k \tag{2.1}$$

and a set $C^i{}_{jk}$ defines a Lie product iff

$$C^k{}_{[ij]} = 0 \text{ and } C^l{}_{[ki} C^m{}_{j]l} = 0 \tag{2.2}$$

are fulfilled, [ ] denoting antisymmetrization. The set of those $C^k{}_{ij}$ that fulfill Eqs. (2.2) form a subset W_n of R^m, $m = n^3$. But W_n is not yet G_n because different points of W_n may describe the same Lie algebra. If this takes place we call the points of W_n to be equivalent and denote this equivalence relation by Q. Then we get the algebraic result[9]

$$G_n = W_n/Q. \tag{2.3}$$

Now we define τ to be the topology in G_n which follows from Eq. (2.3) as quotient topology where W_n is endowed with the topology induced from R^m. As can be seen, τ is naturally defined using Euclidean topologies and quotient spaces only.

As an illustration, let us show the result for $n = 2$: W_2 is homeomorphic to R^2 where the origin, $C^i{}_{jk} = 0$, corresponds to the commutative Lie algebra I, and all other points correspond to the noncommutative one X. Hence $G_2 = (\{I,X\}, \tau)$ and $\{X\}$ is the only nontrivial open set, i.e., $X \to I$ is the only nontrivial converging sequence.

I is the group of translations of the Euclidean plane R^2, whereas X can be represented as a group of linear transformations $x \to ax + b, a > 0$ of the real line R. We denote it by X to avoid confusion with one of the Bianchi types.

For $n \geqslant 3$, we have to specify the equivalence relation Q: A change of the basis e_i will be allowed for the same orientation only, for we have the R^n presumed to be oriented. Therefore, the group $\mathrm{SL}(n) = \{A^i{}_j | \det A^i{}_j > 0\}$ is the gauge group acting on W_n and defining Q. With this definition the equivalence classes of Q are automatically connected, and the usual definition with $\mathrm{GL}(n) = \{A^i{}_j | \det A^i{}_j \neq 0\}$ instead of $\mathrm{SL}(n)$ only identifies some pairs of points in G_n. Such pairs of points we call dual ones. Clearly, the commutative Lie algebra is a self-dual one. [Indeed, $\mathrm{GL}(n)$ is the semidirect product $Z_2 \times \mathrm{SL}(n)$, Z_2 being the two-point group, which is a direct one for n odd.]

The action of $\mathrm{SL}(n)$ on W_n is straightforward since the structure constants transform as usual tensors:

$$\tilde{C}^i{}_{jk} = A^{-1}{}^i{}_a A^b{}_j A^c{}_k C^a{}_{bc}.$$

C. Some properties of τ

First of all, let us look at the commutative algebra $I \in G_n$. The following lemma holds.

Lemma 2.1: $\{I\} \subset G_n$ is closed and G_n is the only neighborhood of I, i.e., $\{I\}$ is the only closed one-point set of G_n. Each nonempty closed subset of G_n contains I; G_n is connected and compact.

Proof: Let $U \subset G_n$ be a neighborhood of I. Further, let $g \in G_n \setminus \{I\}$ and $C^i{}_{jk}$ be structure constants for g. A homothetic basis change $e_i \to \lambda^{-1} e_i$, $\lambda > 0$, hence $C^i{}_{jk} \to \lambda C^i{}_{jk}$ can bring $C^i{}_{jk}$ arbitrarily close to 0. Hence, $g \in U$, the remaining is trivial. □

With Lemma 2.1 in mind it suffices to consider only the subspace $F_n = G_n \setminus \{I\}$ and its relative topology. The following lemma holds.

Lemma 2.2: (F_n, τ) is a compact space. It is a Hausdorff space for $n = 2$ only.

Proof: We have to restrict to $W^0_n = W_n \setminus \{0\}$. Then we may further restrict to sets of structure constants fulfilling the normalization condition

$$\sum_{i,j,k=1}^{n} (C^i{}_{jk})^2 = 1, \tag{2.4}$$

which can be attained by a suitable homothetic basis change, restricting $W^0{}_n$ to the compact subset W^n. [That $W^0{}_n \subset R^m \setminus \{0\}$ is closed follows from the fact that it is the zero set of a continuous function (2.2).] Then, $F_n = W^0{}_n/Q = W^n/Q$ is also compact. Also, $F_2 = \{X\}$, and for $n \geqslant 3$, we find always elements $A \neq B$ of F_n fulfilling $A \to B$. □

The direct limit construction for $n \to \infty$ described at the beginning of Sec. II is justified by the following lemma.

Lemma 2.3: The embedding $\otimes R$ of G_n into G_{n+1} is a continuous, but, surprisingly, not a homeomorphic one. An example for $n = 2$: $X \otimes R$ is Bianchi type III $= \mathrm{VI}_1$.

Proof: The direct product with the one-dimensional Lie algebra R is performed by setting $C^i{}_{jk} = 0$ for $n + 1 \in \{i,j,k\}$. This is not a homeomorphic embedding: Let $n = 3$, then $\mathrm{V} \not\to \mathrm{II}$, but $\mathrm{V} \otimes R \to \mathrm{II} \otimes R$. □

The self-dual elements of G_n can be obtained from the following lemma.

Lemma 2.4: The basis change $e_1 \to -e_1$, $e_i \to e_i$, $i \neq 1$, defines a duality relation $\sim$ in G_n. Here $\tilde{g} = g$ means self-duality. Direct products of a self-dual Lie algebra with an arbitrary Lie algebra are self-dual. Also, $C^i{}_{jk}$ describes a self-dual Lie algebra iff there is a basis change $A^i{}_j$ with $\det A^i{}_j < 0$ leaving $C^i{}_{jk}$ invariant.

For practically evaluating the space (G_n, τ) we need a technical lemma.

Lemma 2.5: Let $(g_i)_i \subset G_n$ be a sequence and $g \in G_n$. Further, let $[g_i], [g] \subset W_n$ be the equivalence classes of Q corresponding to g_i and g, respectively. Then the following statements are equivalent: (1) $g_i \to g$ in τ; (2) to each $x \in [g]$ and to each i there exists an $x_i \in [g_i]$ such that $x_i \to x$ in W_n; and (3) there exists an $x \in [g]$ and to each i an $x_i \in [g_i]$ such that $x_i \to x$ in W_n holds.

Proof: The equivalence of (2) and (3) is proved by a simultaneous basis change. The remaining is straightforward using the continuity of the action of $\mathrm{SL}(n)$. □

Remarks: The specially chosen $x \in [g]$ (in Lemma 2.5.3) can be thought to be a kind of normed structure constant. For $n = 3$, the space (G_3, τ) is explicitly evaluated in Ref. 10. The set W^n is compact; now the crucial point is that the group $\mathrm{SL}(n)$ is not a compact group and so the equivalence classes of Q in W^n need not be compact, i.e., closed subsets of it. This is the very reason for the non-Hausdorffness of the topology τ.

D. Canonical basis freedom and rank

Given a set $C^i{}_{jk}$ of structure constants for a Lie algebra $g \in G_n$, the subset $H_g \subset \mathrm{SL}(n)$ of elements leaving $C^i{}_{jk}$ invariant is a closed subgroup of it. The number $k = \dim H_g$ is called the canonical basis freedom for the Lie algebra g. It depends on g, not on the specially chosen $C^i{}_{jk}$. The rank r is the dimension of the Cartan subalgebra, the Abelian subal-

gebra of highest possible dimension; d_l is the dimension of the lth derived algebra d_l^* which is the subalgebra of g defined by $d_0^* = g$ and $d_l^* = \{[f,h] | f \in d_{l-1}^*, h \in g\}$. The unimodular Lie groups are defined by $C^j_{ij} = 0$ which means an identical vanishing of the trace of the adjoint representation. Semisimple compact Lie groups are always unimodular. Finally, let us define the essential dimension n_{ess} of a Lie algebra $g \in G_n$: n_{ess} is the smallest positive number such that g can be represented as the direct product of $n - n_{ess}$ factors R and a Lie algebra of dimension n_{ess}. Of course, $r + n_{ess} \geqslant n + 1$. How these concepts are connected with the topology τ can be seen from the following lemma.

Lemma 2.6: The following subsets of G_n are closed and therefore compact ones: (1) $\{g | g$ unimodular $\zeta\}$, (2) for each natural m the set $\{g | k > m\}$, (3) for each natural m the set $\{g | r > m\}$, (4) for each natural m and l the set $\{g | d_l < m\}$, (5) surprisingly, the set $\{g | n_{ess} < m\}$ need not be closed.

Proof: Subset (1) is trivial as the zero set of a continuous function is always closed. In subset (2), for $g \in F_n$, the set $[g] \subset W^n$ [the set of structure constants for g fulfilling (2,4)] is of the following type: It is homeomorphic to $SL(n)/(H_g \times R)$ R representing the homothetic motions. Therefore g is a topological manifold of dimension $n^2 - k - 1$. Suppose the statement were wrong. Then there would exist a subset of W^n that would be the limit of subsets of lower dimensions, which is impossible. Subset (3) uses the fact that the Grassmann manifold of all m-dimensional linear subspaces of R^n is compact if endowed, e.g., with the Flachsmeyer topology.[11] In subset (4) d_l can be obtained by calculating certain sets of determinants and then the continuous function argument again works. In subset (5) an example for $n = 3$: n_{ess} (III) $= 2$, n_{ess} (II) $= 3$, but III $\to$ II in τ. □

E. The three-dimensional Lie algebras

The six unimodular three-dimensional Lie algebras (= type A in Ref. 2) can be represented as follows: Bianchi type I is the translation group of R^3; II is the Heisenberg group of matrices

$$\begin{pmatrix} 1 & a & b \\ 0 & 1 & c \\ 0 & 0 & 1 \end{pmatrix}.$$

Bianchi types VI_0/VII_0 are the isometry groups of the Minkowski/Euclidean plane $ds^2 = dt^2 \mp dx^2$; VIII/IX are the isometry groups of the surfaces of constant negative/positive curvature. With

$$[e_1,e_2] = n_3 e_3, \quad [e_2,e_3] = n_1 e_1, \quad [e_3,e_1] = n_2 e_2$$

we have for the triples (n_1,n_2,n_3): (0,0,0) for type I, (1,0,0) for type II, $(1,1,\mp 1)$ for types VIII/IX, respectively.

The remaining groups can be characterized as follows, $h > 0$ being a parameter:

VI_h/VII_h by $[e_1,e_2] = e_3 + he_2$, $[e_2,e_3] = 0$,

$$[e_1,e_3] = \pm e_2 + he_3, \quad VI_1 = III;$$

IV/V by $[e_1,e_2] = be_3 + e_2$, $[e_2,e_3] = 0$,

$$[e_1,e_3] = e_3, \quad b = 1 \text{ for IV}, \quad b = 0 \text{ for V}.$$

The details can be seen from Table I, where $u = 1$ for unimodular algebras and $s = 1$ for self-dual ones and $= 0$ otherwise. The subset of self-dual elements in G_3 is neither open nor closed, e.g., it holds VIII $\to VI_0$ and $VI_0 \to$ II. If G_3 were a Hausdorff space, then, of course, the subset of self-dual elements would become closed, but here we have the two limits $VI_0 \to II_L$ and $VI_0 \to II_R$, $\tilde{II}_L = II_R$, $II_L \neq II_R$, indices L and R denoting handiness (chirality) of the basis.

F. Atoms in the space of Lie algebras

Atoms are those elements $g \in G_n$ for which the closure $cl\{g\}$ of $\{g\}$ contains exactly two elements. Of course, these two elements are I and g itself, and all atoms are contained in F_n. For $n = 2$, the only atom is X. Here A_n, the set of atoms in G_n, can be characterized as follows: $A_n = \{g | \{g\} \subset F_n$ is closed$\}$. The following lemma holds.

Lemma 2.7: Let X be a compact T_0 space and $A \subset X$ be the subspace of closed one-point sets. Then X itself is the only open set containing A.

Proof: Suppose $U \subset X$ is an open set containing A. Then $Y = X \setminus U \neq \phi$ is a compact T_0 space. By construction, Y contains no closed one-point sets. We shall show this to be contradictory. To this end we define a partial order in Y by $x < y$ iff $x \to y$, i.e., $y \in cl\{x\}$. By compactness, each increasing chain contains an upper bound (one of its accumulation points). And by Zorn's lemma, there is a maximal element which has to be a closed one-point set because of the T_0 axiom. □

Therefore the following theorem holds.

Theorem 2.1: The set A_n of atoms in G_n has the property that each non-Abelian Lie algebra can be obtained by an arbitrarily small change of the structure constants of an element of A_n. No proper subset of A_n shares this property.

Proof: We apply Lemma 2.2 and Lemma 2.7 with $X = F_n$, $A = A_n$ and use the definition of the topology τ. □

Of course, Theorem 2.1 could also be proved using the special structure of W^n, but we are interested in showing

TABLE I. Properties[12] of the three-dimensional Lie algebras.

	I	II	III	V	VI_0	VI_h, $h \neq 0,1$	VII_0	VII_h, $h \neq 0$, and IV	VIII/IX
n_{ess}	1	3	2	3	3	3	3	3	3
u	1	1	0	0	1	0	1	0	1
s	1	0	1	1	1	1	0	0	0
k	9	6	4	6	4	4	4	4	3
r	3	2	2	2	2	2	2	2	1
d_1	0	1	1	2	2	2	2	2	3
d_2	0	0	1	2	2	2	2	2	3

which topological structures are essential, and this is done by Lemma 2.7.

Theorem 2.1 makes it desirable to get more knowledge about the set A_n. The following theorem holds.

Theorem 2.2: For each $n \geqslant 3$, there exist exactly two atoms.

Proof: $A_3 = \{\text{II}, \text{V}\}$.[10] Let an arbitrary $g \in F_n$ be given by its structure constants $C^k{}_{ij} \neq 0$. Then one can take a system such that at least one of the values $C^B{}_{1A}$, $A,B = 2,\ldots,n$, does not vanish. A basis change $e_1 \to e_1$, $e_A \to \lambda^{-1} e_A$ gives in the limit $\lambda \to \infty$ a survival of the values $C^B{}_{1A} = -C^B{}_{A1}$ only. The Jacobi identity is then automatically satisfied.

Case (1): $C^B{}_{1A}$ is a multiple of the unit matrix. Then by a transformation $e_1 \to \mu\, e_1$ (and, additionally $e_2 \to -e_2$ if $\mu < 0$), one gets $C^B{}_{1A} = -C^B{}_{A1} = \delta^B{}_A$, the remaining components vanish. There we are arrived at the pure vector type Lie algebras which are somewhat dual to the unimodular ones: We define a Lie algebra to be of a pure vector type if there exists a vector $v_i \neq 0$ such that

$$C^k{}_{ij} = 2v_{[i}\delta^k{}_{j]} \tag{2.5}$$

holds. By contraction, $v_i = C^j{}_{ij}/(n-1)$ and pure vector types are defined by the vanishing of

$$D^k{}_{ij} = C^k{}_{ij} - 2(\delta^k{}_{[j}C^l{}_{i]l})/(n-1). \tag{2.6}$$

For a given n all pure vector type Lie algebras are isomorphic, we donote it by $V^{(n)}$; v_i can be brought to be e_1. We have to show that this algebra is an atom: It is the only type with $C^k{}_{ij} \neq 0$ and $D^k{}_{ij} = 0$. Another proof of this statement is as follows: Let us calculate the subspace $[V^{(n)}] \subset W^n$; it has the topology of the $(n-1)$-dimensional compact sphere S^{n-1}, and in a Hausdorff space, a compact subset is always closed. And why is it S^{n-1}? A basis transformation changes only v_i, and normalization brings it to $|v_i| = 1$, and $S^{n-1} = \{v_i / |v_i| = 1\} \subset R^n$.

Case (2): $C^B{}_{1A}$ is not a multiple of the unit matrix. At this point we need the presumption $n \geqslant 3$. Then one can get $C^3{}_{12} = 1$. A basis change $e_2 \to e_2$, $e_p \to \lambda e_p$, $p = 1,3,\ldots,n$, gives in the limit $\lambda \to \infty$ a survival of elements $C^p{}_{12}$, $p \geqslant 3$, only. For $p \geqslant 4$, an analogous limit gives the following result: The only nonvanishing structure constants are $C^3{}_{12} = -C^3{}_{21} = 1$, which is Bianchi type II $\otimes R^{n-3}$, denoted by $\text{II}^{(n)}$. It is the only possible candidate for a unimodular atom. But Lemma 2.6.1 together with Lemma 2.7 shows that there exists at least one unimodular atom. □

From the above theorem we can see the following simple facts: The noncommutative unimodular Lie algebras form a connected closed compact subset of F_n, and for each unimodular Lie algebra $g \in F_n$, $g \to \text{II}^{(n)}$ holds; $n_{\text{ess}}(\text{II}^{(n)}) = 3$ independently of n, $V^{(2)} = X$, and atom $\otimes R$ need not be an atom! Also, $n_{\text{ess}}(V^{(n)}) = n$.

Contrary to the case of G_n, the question of whether F_n is connected is not at all trivial, because the Jacobi identity imposes quadratic conditions to the definition of W_n, and the connectedness properties of W^n are not clear from the beginning. But the following Theorem holds.

Theorem 2.3: F_n is connected.

Proof: For $n = 2$ it is trivial. Let $n \geqslant 3$. It suffices to give an example of an element g fulfilling $g \in F_n$, $g \to \text{II}^{(n)}$, and $g \to \text{V}^{(n)}$. For $n = 3$, g is then uniquely defined to be IV. Therefore we should find the higher-dimensional analog to Bianchi type IV: It is $\text{IV}^{(n)}$ defined by $[e_1,e_2] = e_2 + e_3$, $[e_1,e_A] = e_A$, $[e_A,e_B] = 0$, for all $A,B \geqslant 3$, $[e_2,e_3] = 0$. □

In U_3, the space of three-dimensional unimodular Lie algebras, VIII and IX are the only isolated points. Moreover, VIII, IX is the smallest dense subset of U_3. This gives a precise meaning to the statement "Bianchi types VIII and IX are the generic unimodular Lie groups" sometimes found in discussions of cosmological models.[13]

III. GEROCH'S LIMIT

Geroch defined[7] in 1969 a limit of space-times: he assigns to a one-parameter set $(M_\lambda)_\lambda$ of space-times M_λ one (or more, not necessarily Hausdorff) limit space. His construction uses neither dimension nor signature of the space-times and is easily generalized to arbitrary dimensions and signatures. Then also his Theorem 1: "Each limit has a maximal extension which is also a limit of that sequence" keeps valid. He gives two equivalent approaches. The first is by embedding his set into a five-dimensional manifold. But it turned out that this is not a true five-dimensional construction because coordinate transformations mixing with the fifth coordinate do not appear. The second approach is by defining families of frames in the space-times M_λ. We prefer to follow this second line of reasoning. The main reason for doing so is the fact that this second approach does not restrict the construction to real values λ but, moreover, can be formulated for denoting the general element of a Moore–Smith (MS) sequence. MS sequences subsume ordinary sequences, real valued index sets, and many other ones. We use them because it is not clear at the moment whether the presumptions on the topology to be defined by ordinary sequences already are fulfilled or not. This makes it possible to define a topology σ in the space of space-times by the condition that a set F is closed iff each Geroch limit of MS sequences contained in F is also an element of F. (Let us remark without proof that Geroch's limit is topological, i.e., the topology σ defines the same convergence as the Geroch limit does.)

Geroch gives an example of a sequence $(M_\lambda)_\lambda$ possessing two limits, one of them being flat space-time. This is a typical result for sequences of asymptotically flat space-times (as the example consists of), because it depends on the coordinates: If the origins of the coordinate systems (i.e., the reference points p_λ, see below) go to infinity quickly enough we get flat space-time as a limit space.

A. The global definition

Now, it is time to give the precise definition of Geroch's limit, generalized to the extent sketched above: Let $(M_\lambda)_\lambda$ be a Moore–Smith sequence of connected Hausdorff C^∞-Riemannian manifolds of the same dimension $n \geqslant 1$ and same signature of the metric g_{ij}, $\det g_{ij} \neq 0$. A connected (not necessarily Hausdorff) C^∞-Riemannian manifold M of dimension n is called a limit space of this sequence if to each $p_0 \in M$ and orthonormal base $(e^0{}_1,\ldots,e^0{}_n)$ at a neighborhood U of p_0 and to each λ there exist points $p_\lambda \in M_\lambda$, orthonormal bases $(e^\lambda{}_1,\ldots,e^\lambda{}_n)$ in neighborhoods U_λ of p_λ such that the metric

components in the U_λ converge to those in U. We require this limit to hold for the metric and all its derivatives uniformly on compact neighborhoods. This ensures the limit of an Einstein space to be automatically an Einstein space, etc.

Example: Let M_λ be the sphere S^2 with a metric of constant curvature and the radius $= 1/\lambda$. In the limit $\lambda \to 0$ one expects to get a plane.[14] More precisely the following holds: There exists an uncountably infinite set of maximal extensions of limits each of which is a flat plane R^2. Of course, they are all equivalent in the sense that they go one into another by a simultaneous rotation of the spheres.

B. The local point of view

The above example shows that at least for homogeneous spaces, globally no essential news appears because the different choices of the p_λ can be called back by isometries of the M_λ. To be accurate, we define a local property as follows: Let (M,p) be such that $p \in M$ and M is a C^∞-Riemannian manifold. Then a geometric property of (M,p) is called a local one if it is a property of each neighborhood $U \subset M$ of p. The pair (M,p) will be called a local Riemannian manifold. Clearly, for homogeneous spaces M, all the pairs (M,p) are equivalent.

Now, we consider Geroch's limit of local Riemannian manifolds. With regard to Hausdorffness we have omitted the possibilities of having two limits by using asymptotically flatness (Geroch's example) as well as by different global topologies ($S^2 \to R^2$), and we can formulate the following theorem.

Theorem 3.1: (1) For local Riemannian manifolds with definite signature, Geroch's limit defines a Hausdorff topology σ.

(2) For indefinite signature this topology is not even T_1.

Proof: (1) Let (M_λ, p_λ) be a sequence of local Riemannian manifolds with definite signature of the metric. We have to show that this sequence possesses at most one limit. Let $E^\lambda = (e^\lambda{}_1,\ldots,e^\lambda{}_n)$ and $F^\lambda = (f^\lambda{}_1,\ldots,f^\lambda{}_n)$ be two sets of orthonormal n-beins at $p_\lambda \in M_\lambda$. For each λ, the basis change matrix from E^λ to F^λ is an element $g_\lambda \in \mathrm{SO}(n)$. The group $\mathrm{SO}(n)$ is compact and therefore, the sequence $(g_\lambda)_\lambda$ contains a convergent subsequence whose limit gives the required basis change from E^0 to F^0.

(2) For Lorentz signature, we have, of course, the Lorentz group instead of $\mathrm{SO}(n)$, and that group is not compact. The required counterexample is the following: Let (M_λ, p_λ) be the same for each value λ, $p_\lambda = (0,0,0,0)$,

$$ds^2 = \cos^2 u\, dx^2 + \cosh^2 u\, dy^2 + 2\, du\, dv. \qquad (3.1)$$

We show the sequence (M_λ, p_λ) to possess two different limits. Of course, one of them is the space itself. It is a nonflat space-time. To get the second limit we perform the coordinate transformation

$$x \to x,\ y \to y,\ u \to u/\lambda,\ v \to v \cdot \lambda.$$

This transformation leaves invariant the metrical tensor

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

but the corresponding sequence of Lorentz transformations has no accumulation point. In the limit $\lambda \to 0$ we get flat space-time. □

Remark: Metric (3.1) is a plane wave solution of Einstein's vacuum field equation and the property shown here holds for all of its points. On the other hand, each polynomial curvature invariant of arbitrary order (all of them are local invariants) uniquely converges, from which we can see without any calculations that all these invariants identically vanish for metric (3.1). This latter property is connected with the existence of a nontrivial homothetic motion with regular fixed point. Next, let us concentrate on homogenous Riemannian spaces.

IV. THE SPACE OF HOMOGENEOUS RIEMANNIAN SPACES

In this section we shall give some relations between the Geroch limit in the set of homogeneous Riemannian spaces of definite signature and the topology τ in the set of the respective Lie groups of isometry. Let us first note a result of Geroch[7]: "Let each element of a sequence of space-times possess a k-dimensional group of motions then so does its limit. Also the existence of a hypersurface-orthogonal Killing vector is hereditary." The question, however, of which groups can appear in the limit remained unsolved in that paper, and we go on that way.

In both cases we consider the local properties only, thus we consider only the spaces (G_n, τ) of Lie algebras of dimension n (cf. Sec. II) and the spaces (N_n, σ) of homogeneous local Riemannian spaces of dimension n and positive definite metric with Geroch's limit (cf. Sec. III).

By Theorem 3.1, (N_n, σ) is a Hausdorff space. Also N_2 is homeomorphic to the real line, it can be uniquely parametrized by the curvature scalar R. All homogeneous Riemannian spaces are automatically analytical ones and we have no problems with differentiability classes. The following lemma holds.[6]

Lemma 4.1: To each n there exists a number $m(n)$ such that the set $\{I_1,\ldots,I_{m(n)}\}$ of all $m(n)$ polynomial curvature invariants up to a certain order gives a unique parametrization of N_n. Moreover, this embedding $(N_n,\sigma) \subset R^{m(n)}$ is a homeomorphic one.

Remark: A polynomial invariant of degree k and order l is a linear combination of monoms

$$g^{j_1 i_2} \cdots g^{i_{2k-1} i_{2k}} R_{j_1 j_2 j_3 j_4 j_5 \cdots j_{l+4}} R_{j_{l+5} \cdots} \cdots,$$

with $(j_1,\ldots,j_{2k})$ being a permutation of $(i_1,\ldots,i_{2k})$, l denotes the maximal number of covariant derivatives of the curvature tensor R_{ijkl}.

Proof: For the first part compare MacCallum,[6] continuity of the embedding is trivial, inverse continuity follows from local compactness. □

A. Simply transitive groups of motion

In this first step we consider the subspace $K_n \subset N_n$ of those homogeneous local Riemannian spaces whose isometry group possesses a simply transitive subgroup. Here $K_2 = N_2$, and $N_3 \setminus K_3$ contains only the homogeneous $S^2 \otimes R$, i.e., the Kantowski–Sachs model. The elements of K_n can be

obtained as follows: Take a Lie algebra $g \in G_n$, fix the structure constants $C^i{}_{jk}$ and the metric $g^0{}_{ij}$ at one point and then calculate the full g_{ij} by left translation via the given Lie group.[15] By a basis change we can always get $g^0{}_{ij} = \delta_{ij}$, and the pair $(C^i{}_{jk}, \delta_{ij})$ uniquely defines the homogeneous local Riemannian space. Thus we have a map

$$\pi: W_n \to K_n. \tag{4.1}$$

The following theorem holds.

Theorem 4.1: The map π is continuous and surjective.

Proof: Each polynomial curvature invariant is a polynomial in the numbers $C^i{}_{jk}$ (cf. Ref. 2) and then by applying Lemma 4.1. "π is onto" follows directly from the definition of K_n. □

Equation (4.1) defines an equivalence relation Iso in W_n:

$$C^i{}_{jk} \text{ Iso } C'^i{}_{jk} \text{ iff } \pi(C^i{}_{jk}) = \pi(C'^i{}_{jk}),$$

i.e., structure constants are Iso equivalent iff the corresponding Riemannian spaces are locally isometrically diffeomorphic. Iso is the operation of forgetting the Lie group origin in the pair (Lie group, left invariant metric) only preserving the metric. Of course, the original Lie group reappears as subgroup of the isometry group.

The equivalence relations Q (cf. Sec. II) and Iso in W_n are not comparable: $C^i{}_{jk}\ Q\ \lambda C^i{}_{jk}$, but the corresponding curvature scalars differ by a factor λ^2, hence, they are in general not isoequivalent. On the other hand, take a Riemannian manifold V_3 of constant negative curvature then one has simply transitive subgroups of both Bianchi types V and VII_h, thus isoequivalence does not necessarily imply Q equivalence. The isoequivalence classes in W_n will be denoted by $\langle x \rangle$. Consequently, $\langle I \rangle = \{I\}$ corresponds to flat space.

One main relation between (G_n, τ) and (K_n, σ) is given by the following theorem.

Theorem 4.2: Let $(g_i)_i$, $g \in G_n$, with $g_i \xrightarrow{\tau} g$. Let $V \in K_n$ possess g as a simply transitive subgroup of its isometry group, then there exists a sequence $(V_i)_i \subset K_n$ such that for each i, g_i is a simply transitive subgroup of the isometry group of V_i which fulfills $V_i \xrightarrow{\sigma} V$.

Proof: Fix a basis and the metric at the origin for V and then vary the structure constants according to *Lemma* 2.5. The remaining follows from the definitions of σ and τ. □

Analogously to $F_n \subset G_n$ we define, justified by Lemma 4.1,

$$L_n = \left\{ x \in K_n \,\middle|\, \sum_{i=1}^{m(n)} (I_i)^2 = 1 \right\}, \tag{4.2}$$

i.e., L_n contains—up to a homothetic transformation—all nonflat elements of K_n. Indeed, the following lemma holds.

Lemma 4.2: $L_n \otimes R = K_n \setminus \pi(I)$ is a homeomorphism, "$\otimes R$" denotes the homothetic map.

Now, from a first glance, comparing Theorem 4.1 with Lemma 2.2 [Eq. (4.2) is analogous to Eq. (2.4)] one could expect L_n to be a compact space, referring to the fact that the continuous image of a compact space is itself compact. L_2 is the two-point space, but already L_3 is not compact: The closure of L_3 in N_3 adds exactly one point to it. It corresponds to the normed Kantowski–Sachs model as limit of a sequence of models of Bianchi type IX.

B. Multiply transitive groups of motion

At least this last fact shows the necessity to consider multiply transitive groups of motion for larger values of n: One should take a Lie algebra g of dimension $d \geqslant n$ and a subalgebra $h \subset g$ of codimension n. Then a metric should be fixed at the origin of g/h that is invariant with respect to h, and then again transported by left translations to all g/h. For $d > n$, the Ricci tensor cannot possess n different eigenvalues. The possible values of d are n, $n+1$, ..., $n(n+1)/2-2$, and $n(n+1)/2$, for h is a subalgebra of $\text{SO}(n)$. But $n = 3$ is a case where the appearance of multiple transitive groups of motion without simply transitive subgroups is only one singular case and we will concentrate on comparing (G_3, τ) with (N_3, σ).

We can simply generalize Lemma 4.2 as follows.

Lemma 4.3: Let $L_n^* = \{x \in N_n \mid \Sigma I_i^2 = 1\}$ then $L_n^* \otimes R = N_n \setminus \pi(I)$ is a homeomorphism.

C. Complete comparison for $n=3$

In this section we prove some relations between the Lie algebras (G_3, τ) and the locally homogeneous Riemannian spaces (N_3, σ). To give the concept "convergence to a subgroup" a precise meaning we define the following: Let $G^n = \cup_{m=1}^n G_m$. The topology τ^* in G^n is defined as follows: Let $g \in G^n$, i.e., $g \in G_m$ for a certain $m \leqslant n$. Let $H(g)$ be the set of subalgebras of g and for each $h \in H(g)$ let U_h be a τ neighborhood of h. Then the sets $U^*(g) = \cup_{h \in H(g)} U_h$ form a base for the topology τ^* in G^n. Then $g_i \xrightarrow{\tau^*} g$ in G^n means: "$(g_i)_i$ τ-converges to a subalgebra of g." The omission of an index n at τ^* is justified by Lemma 4.3. The identical embedding of G^{n-1} into G^n is a τ^*–τ^*-homeomorphic one with an open image, and τ^* restricted to one $G_m \subset G^n$ just gives τ. Let $h_i \xrightarrow{\tau} h \subset g$ then $h_i \xrightarrow{\tau^*} g$.

Now we can formulate the complement to Theorem 4.2.

Theorem 4.3: The space N_3 of all three-dimensional locally homogeneous Riemannian manifolds with positive definite metric is a three-dimensional topological manifold with boundary. Let $V_i \to V$ converge in (N_3, σ). Then the isometry groups of the V_i τ-converge to a subgroup of the

Proof: The proof is lengthy but straightforward, we sketch the essential steps only. First, let V be flat space, one of the boundary points of N_3. Then the statement follows from the definition of τ independently of the special structure of the V_i, cf. Lemma 2.1. Second, let V be nonflat. By Lemma 4.3 we may restrict to L_3^* instead of N_3. Let us illustrate the calculation for the Bianchi type IX: the general line element reads[2]

$$ds^2 = a(\cos y \cos z\, dx - \sin z\, dy)^2 + b(\cos y \sin z\, dx + \cos z\, dy)^2 + c(dz - \sin y\, dx)^2. \tag{4.3}$$

The eigenvalues of the Ricci tensor R_{ij} for metric (4.3) are

$$(\lambda,\mu,\nu) = (2abc)^{-1}(a^2-(b-c)^2,$$
$$b^2-(a-c)^2,\ c^2-(a-b)^2). \qquad (4.4)$$

Two such metrics are isometrically diffeomorphic iff one of the triples (a,b,c) is a permutation of the other. (If we insisted on oriented spaces this permutation would be restricted to be an even one, but we do not insist on them.) We have a four-dimensional group of motions in (4.3) iff two of the three values a,b,c coincide and these points form the boundary; $a=b=c$ gives the isotropic space, it forms an edge[16] in L_3. The limits of the spaces (4.3) we get by taking the Geroch limit with suitably chosen $a,b,c\to 0$, a finite value, or ∞ such that all values (4.4) remain finite. Then one can see that only Bianchi types VII_0, II, I and the Kantowski–Sachs models appear as limits as must be the case.

Within L_3, Bianchi types VIII and IX form two-dimensional subsets, II and V form single points and all other types form one-dimensional subsets. Therefore, the space is topologically three-dimensional and —up to a zero set—locally Euclidean. □

In spite of its three dimensionality we can prove the following theorem for N_3.

Theorem 4.4: Let L,M,N be three polynomial curvature invariants. Then there exist different points of N_3 with the same triple (L,M,N).

Corollary: The three invariants

$$R,\ R_{ij}R^{ij},\ R_{ij}R^{jk}R_k{}^i \qquad (4.5)$$

do not suffice for a unique characterization of the three-dimensional locally homeomorphic Riemannian manifolds of positive signature.

Example: The invariants (4.5) are in one-to-one correspondence to the invariants (4.4). In general, a,b,c can be (up to a permutation) calculated from λ, μ, and ν. But for $\lambda>0$, $\mu=\nu=0$, we have only $a=b+c$ and one relation between b, c, and λ to be fulfilled, thus a one-parameter set of spaces with the same invariants (4.5). The Cotton-York invariant $R_{i[j;k]}R^{i[j;k]}$ parametrizes this set.

Proof of Theorem 4.4: It suffices to show that N_3 cannot be homeomorphically embedded into the R^3. Bianchi type VII_0 gives a two-dimensional subset A of N_3. For an open dense subset of A, all three Ricci tensor eigenvalues are different, thus in a σ neighborhood of these points, we do not have a four-dimensional group of isometries, i.e., not a mixing of different Bianchi types. By Theorem 4.2, each point of A is the limit of a one-parameter set of spaces of Bianchi type VIII, another one-parameter set of Bianchi type IX, and a third one-parameter set of type VII_h, $h>0$, $h\to 0$. And this triangle structure around A cannot be embedded into the R^3. □

Some further properties of N_3 (cf. also Ref. 5) can be seen from the following.

Theorem 4.5: Let $w\neq 0$, then the following holds: If the Ricci tensor eigenvalues of a locally homogeneous Riemannian V_3 of positive signature (i.e., an element of N_3) are (1) w,w,w, then the space is of constant curvature; (2) $0,w,w$, then it is the Cartesian product of a line with a plane of constant curvature; and (3) $0,0,w$, then it is Bianchi type VIII (for $w<0$) or Bianchi type IX (for $w>0$). For each fixed value w, one has a one-parameter family of spaces. If (4) $w,-w,-w$ with $w>0$, then it is Bianchi type II; and (5) $0,w,-w$ and some other triples do not appear in N_3.

D. Partial results for $n>4$

We have proved Theorems 4.3 and 4.5 by calculating a complete list of examples for all the possible changes between the nine Bianchi types. Thus to generalize them to arbitrary dimensions n requires another method of proving.[17] Now we look for the homogeneous local Riemannian spaces corresponding to the atoms and isolated points of G_n for arbitrary values n. The following theorem holds.

Theorem 4.6: Let $g\in G_n$ be an n-dimensional Lie algebra and $B_g\subset N_n$ be the set[18] of local homogeneous Riemannian spaces possessing g as a simply transitive subgroup of their isometry group. Then the following holds: (1) g is an atom iff $B_g\cap L_n$ consists of exactly one point; (2) g is an atom iff B_g is a closed nonempty subset of $(N_n\setminus\{\text{flat space}\},\sigma)$; (3) for $g=V^{(n)}$, $n\geqslant 2$, B_g is the set of spaces of constant negative curvature; (4) for $g=\mathrm{II}^{(n)}$, $n\geqslant 3$, B_g consists of spaces whose Ricci tensor eigenvalues are $w,-w,-w,0,\ldots,0$ with $w>0$; and (5) g is an isolated point iff B_g is an open subset of K_n. This means that for the isolated Lie groups, perturbing a homogeneous space to another homogeneous space of K_n cannot change the type if the perturbation is sufficiently small.

Proof: (3) follows from explicit calculations with the structure constants implying the validity of (1) and (2) for atoms g, cf. Theorem 2.2. Let us show (1) and (2) with g not being an atom. Here $g=I$ implies $B_I=$ flat space, $g\neq I$, g not an atom implies $g\to h$, $h\in G_n$, h atom. Then apply Theorem 4.2. Statement (4) can be calculated explicitly, cf. the end of Sec. II F, or Ref. 15a. □

Corollary: For each $n\geqslant 3$, there exists a one-parameter subset $x(\lambda)\subset L_n$, $0\leqslant\lambda\leqslant 1$, with $x(0)$ representing type $V^{(n)}$, $x(1)$ representing type $\mathrm{II}^{(n)}$, and for each $0<\lambda<1$, $x(\lambda)$ belongs to type $\mathrm{IV}^{(n)}$. For $n=3$, all spaces of Bianchi type IV have three different Ricci tensor eigenvalues; and all spaces of Bianchi type IV belong to that curve $x(\lambda)$.

V. DISCUSSION

In the present paper we have continued the discussion[10] of how the Bianchi type can change with time in an intrinsically homogeneous cosmological model. A direct change from type A to type B [$V_3(t)$ is of type A for $t<0$, type B for $t=0$] is possible iff $A\xrightarrow{\tau}B$, cf. the diagram.[10] Here we generalized most of the results to higher dimensions and pointed out relations to Geroch's limit of space-times on the one hand and to general topological properties on the other hand.

One application is already performed in Ref. 19: For deriving the Einstein field equation (or other equations) for homogeneous cosmological models one has to derive them only for a τ-dense subset of G_3 (here: Bianchi types VI, VII, VIII, and IX). The equations for the other types follow then simply from a limiting procedure. Also for the corresponding solutions it holds: Let $A\to B$. If a σ-converging sequence[20] of type A solutions gives a limit belonging to type B, then this is also a solution. But, in general, not all type B

solutions will be obtained by this procedure.

Example: Let A denote spherical, and B denote plane symmetry.[21] But plane wave solutions of Einstein's equation are not limits of the Schwarzschild solution.[22]

Now, consider the Schrödinger equation (or another one) in a potential $V_0(\mathbf{x})$ possessing the symmetry Lie group g_0. Then consider a perturbation $V_\lambda(\mathbf{x})$ with symmetry group g_λ. Then the g_λ τ-converge to a subgroup[23] of g_0 as $\lambda \to 0$, but the g_λ themselves *need not* be subgroups of g_0. Maybe this fact is connected with (accidental) degeneration of energy levels in perturbation problems. Also for the subgroup structure in GUT models the topology τ has possibly a relevance.

One should also search for connections of the topology τ to the respective global topologies of the Lie groups and homogeneous Riemannian spaces. Compare Ref. 24 for the topologies of globally homogeneous spaces. Not only the structure constants but also the finitely many generators of the homotopy group continuously change.

APPENDIX[25]: TOPOLOGY AND SEPARATION AXIOMS

A topological space is a nonempty set X and a set $\mathfrak{U}$ of subsets of X. The elements of $\mathfrak{U}$ are called open sets (a generalization of the open intervals in the real line). One requires $\{\phi, X\} \subset \mathfrak{U}$ (trivial open sets), $\{X, Y\} \subset \mathfrak{U}$ implies $X \cap Y \in \mathfrak{U}$ and $\{X_i | i \in L\} \subset \mathfrak{U}$ implies $\cup_{i\in L} X_i \in \mathfrak{U}$ (finite intersections and arbitrary unions of open sets are open). A sequence $(x_i)_{i\in L} \subset X$ is called to converge to a limit point $x \in X$, $x_i \to x$, iff to each $U \in \mathfrak{U}$ fulfilling $x \in U$ (hence, U is a neighborhood of X) there exists an i_0 such that for all $i > i_0$, $x_i \in U$ holds. Thereby, L is a partially ordered set, e.g., the naturals. The main separation axioms T_n (T from German *Trennung*) are defined as follows: X is T_0 iff each pair of points can be weakly separated, i.e., there exists an open set containing only one of both. This axiom is usually required to be fulfilled; X is T_1 iff each pair of points has open neighborhoods whose intersection does not contain any of them. Equivalently, X is T_1 iff each one-point set is closed, i.e., the complement of an open set; X is T_2 iff each pair of points can be separated, i.e., they possess disjoint open neighborhoods. This is the Hausdorff axiom. Clearly, T_n implies the validity of T_{n-1}. The axioms $T_{0,1,2}$ can be equivalently characterized as follows: X is T_2 iff each sequence has at most one limit; X is T_1 iff each constant sequence has at most one limit. If all x_i are equal to y we write simply $y \to x$ instead of $x_i \to x$; X is T_0 iff to each pair of points there is a sequence converging only to one of them.

A topological space X is called to be compact, iff to each system $\mathfrak{A} \subset \mathfrak{U}$ with $\cup_{\mathfrak{U}\in\mathfrak{A}} \mathfrak{U} = X$ there exists a finite subset $\{U_1, \ldots, U_n\} \subset \mathfrak{A}$ with $\cup_{i=1}^n U_i = X$. (Each open cover contains a finite subcover.) Equivalently it holds that X is compact iff to each sequence in X there exists a converging subsequence. (Each sequence has an accumulation point.)

Example: Let X be a T_0 space and $x \in X$ such that X is the only open neighborhood of x. Then X is compact and x is an accumulation point of all sequences.

A topological space X is called to be connected iff U, $V \in \mathfrak{U}$, $U \cup V = X$ implies $U \cap V \neq \emptyset$.

If Q is an equivalence relation in X then the quotient topology in the quotient space X/Q is defined as follows: A set of equivalence classes is open in X/Q iff their union is open in X. Of course, the quotient space of a compact space is compact. The associated T_0 space of X is the space X/Q, where xQy holds iff both $x \to y$ and $y \to x$.

[1] L. Bianchi, Soc. Ital. Sci. Mem. Mat. **11**, 267 (1897), for dimension $n = 3$; J. Schell, J. Math. Phys. **2**, 202 (1961), for $n = 4$.

[2] D. Kramer, H. Stephani, M. MacCallum, and E. Herlt, *Exact Solutions of Einstein's Field Equations* (Wissenschaften, Berlin, 1980).

[3] See also Sec. II E for a definition of the Bianchi types.

[4] C. Collins and D. Szafron, J. Math Phys. **20**, 2347 (1979); H.-J. Schmidt, Astron. Nachr. **303**, 283 (1982); T. Wolf, Ph. D. thesis, Jena University, 1986 (unpublished).

[5] D. Szafron, J. Math. Phys. **22**, 543 (1981).

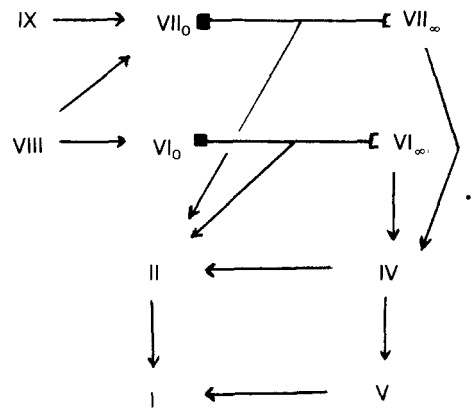
[6] This is a special case of the equivalence problem for Riemannian spaces, cf., e.g., A. Karlhede and M. MacCallum, Gen. Relativ. Gravit. **14**, 673 (1982); and M. MacCallum, in *Classical General Relativity*, edited by W. Bonnor, J. Islam, and M. MacCallum (Cambridge U. P. Cambridge, 1984), p. 145.

[7] R. Geroch, Commun. Math. Phys. **13**, 180 (1969).

[8] For an application of Geroch's limit to the Wahlquist solution see D. Kramer, GR 11-Abstracts 260 (International Society for General Relativity and Gravitation, Stockholm, 1986).

[9] Up to this point cf. W. Roque and G. Ellis, *Galaxies, Axisymmetric systems and Relativity* edited by M. MacCallum (Cambridge U.P., Cambridge, 1985), p. 54.

[10] H.-J. Schmidt, Astron. Nachr. **303**, 227 (1982). The properties of (G_3, τ) can be seen from the diagram. $\mathrm{VI}_h \to \mathrm{II}$ holds for each h and $\lim_{n\to\infty} \mathrm{VI}_{h_n} = \mathrm{IV}$ implies $\lim_{n\to\infty} h_n = \infty$:



[11] J. Flachsmeyer, Math. Nachr. **26**, 321 (1963); cf. also H.-J. Schmidt, *ibid.* **104**, 271 (1981).

[12] The lines "s" and "n_{css}" seem to be original, the remaining cf., e.g., Ref. 2.

[13] See, e.g., G. Ellis and M. MacCallum, Commun. Math. Phys. **12**, 108 (1969).

[14] A. Krasinski, Gen. Relativ. Gravit. **13**, 1021 (1981) applies such a limit to a generalized Friedman cosmological model.

[15] Cf. (a) J. Milnor, Adv. Math. **21**, 293 (1976) for curvatures of left invariant metrics on Lie groups; (b) J. E. D'Atri and W. Ziller, Mem. A.M.S. **18**, 215 (1979), for Einstein metrics on compact Lie groups.

[16] Here one can geometrically see how the spaces with higher symmetries are characterized as points without Euclidean neighborhood. This is quite analogous to the linearization stability results of A. Fischer, J. Marsden, and V. Moncrief, Ann. Inst. H. Poincaré **33**, 147 (1980).

[17] If additionally the space V is supposed to possess n different Ricci tensor eigenvalues, Theorem 4.3 remains valid for arbitrary n, because for that case, no higher-dimensional isometry group appears.

[18] $\dim B_g \leqslant n(n+1)/2$, and $g \to h \in G_n$ implies $\dim B_g \geqslant \dim B_h + 1$.

[19] V. Müller and H.-J. Schmidt, Ann. Phys. (Leipzig), in print.

[20] The full space-time being considered as dynamical system with a topology analogous to σ cf. K. Kuchař, J. Math. Phys. **17**, 777 (1976); cf. also the ideas of the world function of the universe, S. Hawking and Z. Wu, Phys. Lett. B **151**, 15 (1985).

[21] J. Horský and J. Novotný, in Czech. J. Phys. B **32**, 1321 (1982) consider the analogy between the plane and the spherical solutions of Einstein's equation from the particle's motion point of view. M. Carmeli and C.

Charach, in Phys. Lett. A **75** 333 (1980) consider a sequence of solutions of Bianchi type VI_h, converging to a solution of type V for $h \to \infty$. A. Spero and R. Baierlein, in J. Math. Phys. **19**, 1324 (1978) define approximate symmetry groups of inhomogeneous metrics. I suppose that this group is also σ–τ-continuous in the space of space-times.

[22]A nontrivial example for the topology σ in a space of solutions is given in V. Müller and H.-J. Schmidt, Gen. Relativ. Gravit. **17**, 769 (1985): For the Lagrangian $L = R + m R^2$, R being the curvature scalar, the space of all nonflat spatially flat Friedman cosmological vacuum models is a circle S^1 for $m < 0$ (no tachyons) and the real line with one double point (hence a T_1 but not a Hausdorff space) for $m > 0$.

[23] I. Protatsov and Ju. Tsibenko, in Dokl Akad. Nauk Ukrain SSR, Ser. A **10**, 77 (1981) consider a topology in the space of subgroups of a topological group; cf. also H.-J. Schmidt, Math. Nachr. **118**, 105 (1984).

[24]M. Osinovsky, Ann. Inst. H. Poincaré **19**, 197 (1973); H. Fagundes, Phys. Rev. Lett. **54**, 1200 (1985).

[25]See, e.g., W. Rinow, *Topologie* (Wissenschaften, Berlin, 1975); J. Kelley, *General Topology* (Van Nostrand, New York, 1957).