Representations and invariant equations of E(3)

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Using methods analogous to those introduced by Gel'fand *et al.* [*Representations of the Rotation and Lorentz Groups and Their Applications* (Pergamon, New York, 1963)] for the Lorentz group the matrix elements for the representations of the Lie algebra of the Euclidean group in three dimensions E(3) are explicitly derived. These results are then used to construct invariant equations with respect to this group and to show, in particular, that the nonrelativistic analog to the Dirac equation is not unique.

I. INTRODUCTION

The Euclidean group in three dimensions E(3) plays in classical mechanics the same role that the Lorentz group plays in relativistic mechanics.[1–3] Moreover, from a mathematical point of view, the Lie algebras of these two groups contain six generators J_i, K_i, $1 = 1,2,3$, whose commutation relations (CR) for the Lorentz algebra are

$$[J_i,J_j] = \epsilon_{ijk}J_k, \tag{1.1}$$

$$[J_i,K_j] = \epsilon_{ijk}K_k, \tag{1.2}$$

$$[K_i,K_j] = -\epsilon_{ijk}J_k. \tag{1.3}$$

The CR of the Lie algebra of E(3) differ from those above only in the third set [Eq. (1.3)], which is replaced by

$$[K_i,K_j] = 0. \tag{1.4}$$

[For more details regarding the generators of E(3) and the notations used for the rest of this paper see the Appendix.]

In view of these similarities it is surprising to find that the representations of these algebras and their respective invariant equations were treated rather differently in the literature.

Thus while complete and explicit expressions for the matrix elements of the irreducible representations of the Lorentz algebra and its invariant equations exist in the literature[4] the same is not true for E(3). As for this latter algebra the "general form" of the matrix elements for the finite (indecomposable) irreducible representations were given (somewhat) indirectly in Ref. 5. What has been left open, however, was the computation of the interlocking constants between the various irreducible representations of O(3) that appear in the decomposition of an E(3) representation (especially when can these interlocking constants be nonzero). These constants can be computed by *ad hoc* methods (as suggested in Ref. 5) only in some very simple cases.

In view of these circumstances it is our first objective in this paper (Sec. II) to derive explicitly, the expressions for the matrix elements for some of the irreducible representations of E(3) (both finite and infinite dimensional) by methods that are completely analogous to those used by Gel'fand *et al.* for the Lorentz group.[4]

In Sec. III we present a systematic approach to the construction of first-order invariant equations with respect to E(3) subject to the constraint that each component of the wave function satisfies the Galilean energy momentum relation $2mE = m^2 + p^2$ (Refs. 6–8). As a result we show that the nonrelativistic analog to the Dirac equation is not unique and that there is no nonrelativistic analog to the Majorana equation.[9]

II. REPRESENTATIONS OF E(3)

To construct the representations of E(3) we first observe that Gel'fand *et al.*[4] already found the most general solution of the CR(1.1), (1.2). Adopting the notations used by Gel'fand *et al.* we can write this solution as follows:

$$H_3\xi^{\tau}_{l,m} = m\xi^{\tau}_{l,m}, \tag{2.1}$$

$$H_+\xi^{\tau}_{l,m} = \alpha^l_{m+1}\xi^{\tau}_{l,m+1}, \tag{2.2}$$

$$H_-\xi^{\tau}_{l,m} = \alpha^l_m\xi^{\tau}_{l,m-1}, \tag{2.3}$$

$$F_3\xi^{\tau}_{l,m} = \sum_{\tau'}\{C^{\tau\tau'}_l d(l,m)\xi^{\tau'}_{l-1,m} - A^{\tau\tau'}_l \times m\xi^{\tau'}_{l,m} - C^{\tau\tau'}_{l+1}\, d(l+1,m)\xi^{\tau'}_{l+1,m}\}, \tag{2.4}$$

$$F_+\xi^{\tau}_{l,m} = \sum_{\tau'}\{C^{\tau\tau'}_l g_1(l,m)\xi^{\tau'}_{l-1,m+1} - A^{\tau\tau'}_l g_2(l,m)\xi^{\tau'}_{l,m+1} + C^{\tau\tau'}_{l+1}g_3(l,m)\xi^{\tau'}_{l+1,m+1}\}, \tag{2.5}$$

$$F_-\xi^{\tau}_{l,m} = \sum_{\tau'}\{-C^{\tau\tau'}_l g_1(l,-m)\xi^{\tau'}_{l-1,m-1} - A^{\tau\tau'}_l g_2(l,-m)\xi^{\tau'}_{l,m-1} - C^{\tau\tau'}_{l+1}g_3(l,-m)\xi^{\tau'}_{l+1,m-1}\}, \tag{2.6}$$

where

$$\alpha^l_m = [(l+m)(l-m+1)]^{1/2},$$
$$d(l,m) = [l^2 - m^2]^{1/2},$$
$$g_1(l,m) = [(l-m)(l-m-1)]^{1/2},$$
$$g_2(l,m) = [(l-m)(l+m+1)]^{1/2},$$
$$g_3(l,m) = [(l+m+1)(l+m+2)]^{1/2}.$$

It is therefore clear that the only step one must take in order to construct the representations of E(3), rather than O(3,1) is to subject this general solution to the constraints given by Eqs. (1.4) rather than those of Eqs. (1.3). To carry this program out we begin by constructing two special types of representations that are important from a physical point of view. There are the following.

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(1) Representations of E(3) whose decomposition with respect to O(3) contains each irreducible representation of O(3) at most once.

(2) Representations of E(3) in whose decomposition with respect to O(3) only one irreducible representation of this group appears (several times).

Case 1: Since each representation of O(3) appears only once in the decomposition we can drop the degeneracy index τ.

Furthermore, we observe that if the representation is irreducible and l_0, l_1 are, respectively, the lowest and highest l's that appear in the decomposition then each l_0+n, $n=1,2,\ldots,l_1-l_0$ must also appear in the decomposition. In fact, if some representation l_0+n is missing then we can infer [since the generators of the algebra, according to (2.1)–(2.5), can connect states of l_0+n-1 only with those of l_0+n and (l_0+n-2)] that the representations $l_0,\ldots,l_0+n-1$ form an invariant subspace in contradiction to the assumption that the representation is irreducible.

Thus an irreducible representation of E(3) that belongs to this class is a "ladder representation" which is either finite or infinite (presently we show that the ladder must be infinite).

To construct these irreducible representations we apply any of the constraints $[F_+, F_3]=[F_+, F_-]=[F_-, F_3]=0$ to Eqs. (2.4)–(2.6) under the present assumptions and obtain the following equations:

$$[A_l(l+1)-A_{l-1}(l-1)]C_l=0, \tag{2.7}$$

$$[A_{l+1}(l+2)-A_l l]C_{l+1}=0, \tag{2.8}$$

$$[2l-1]C_l^2-[2l+3]C_{l+1}^2-A_l^2=0. \tag{2.9}$$

To solve these equations we first observe [using Eqs. (2.4)–(2.6)] that for an irreducible representation $C_{l+1}=0$, only if $l=l_1$ (if such a finite l_1 exists) and similarly $C_l=0$ only if $l=l_0$. Hence for other l's that appear in the decomposition of the representation with respect to O(3), both C_l, C_{l+1} are nonzero and we infer from Eqs. (2.7) and (2.8) that

$$A_l=A_{l-1}(l-1)/(l+1),$$

which leads to

$$A_l=A_{l_0}[l_0(l_0+1)/l(l+1)], \tag{2.10}$$

where A_{l_0} is an arbitrary constant. Furthermore, to complete the analogy with the Lorentz group we rewrite (2.10) in the form

$$A_l=il_0L/l(l+1). \tag{2.11}$$

To evaluate the C_l's we now multiply Eq. (2.9) by $(2l+1)$ and sum the resulting equations for $l=l_0,\ldots,l$. This yields, after some algebra,

$$C_l^2=L^2[(l^2-l_0^2)/(4l^2-1)l^2]. \tag{2.12}$$

We infer from this relation that contrary to the Lorentz group a ladder representation of E(3) must be an infinite-dimensional representation. In fact (2.12) implies that either $C_l=0$ for all l (the representation is then reducible) or $C_l\neq 0$ for all l_0+n, $n=1,2,\ldots$. We thus proved the following.

Proposition 1: All irreducible ladder representations of E(3) are of infinite dimension (except the trivial one-dimensional representation). The matrix elements of these representations are given by Eqs. (2.1)–(2.6), where A_l, C_l are determined by Eqs. (2.11), (2.12), respectively.

It appears to us that the explicit computation of these matrix elements is new.

Case 2: When the decomposition of the representation under consideration with respect to O(3) contains only one irreducible representation l of this group with multiplicity n, then obviously the matrix elements of J_i are given by the Kronecker product

$$J_i=I\times J_i(l), \tag{2.13}$$

where $J_i(l)$ are the matrix elements of the irreducible representation l of O(3) and I is the unit matrix of dimension n. The matrix elements of the other generators of the algebra are given by the following proposition.

Proposition 2: Under the present assumption the matrix elements of K_i are given by

$$K_i=N\times J_i(l), \tag{2.14}$$

where N is an $n\times n$ matrix so that $N^2=0$. Moreover, if N admits an invariant (proper) subspace then the representation is reducible otherwise the representation is indecomposable.[10]

Proof: It is easy to show that if J_i, K_i are given by Eqs. (2.13) and (2.14) then all the CR of the algebra are satisfied.

In fact,

$$[J_i,K_j]=N\times[J_i(l),J_j(l)]=N\times\epsilon_{ijk}J_k(l)=\epsilon_{ijk}K_k$$

and

$$[K_i,K_j]=N^2\times\epsilon_{ijk}J_k=0.$$

To show that this is the only possible solution of the CR under present assumptions it is enough to observe that the matrix elements of K_3 are [using (2.4)]

$$(K_3)^{\tau\tau'}_{l,l,m,m'}=A^{\tau\tau'}m\delta_{m,m'}, \tag{2.15}$$

i.e., $K_3=N\times J_3(l)$.

An appropriate form of the matrix N which is important in the construction of E(3) invariant equations is given by

$$\mathrm{N}=\begin{bmatrix} 0 & & & & \\ \alpha_2 & & & 0 & \\ \vdots & 0 & \ddots & & \\ \alpha_{n-1} & & & & \\ \epsilon,\beta_2 & & \cdots & \beta_{n-1} & 0 \end{bmatrix}, \tag{2.16}$$

where $\alpha_2\beta_2+\cdots+\alpha_{n-1}\beta_{n-1}=0$ and ϵ is an arbitrary parameter.

We now proceed to discuss the irreducible representations of E(3) in the general case, i.e., when the decomposition of the representation with respect to O(3) contains the representations $l_0 l_0+1\ldots,l_1$, each with multiplicity n_i. (Obviously such a representation is irreducible only if all the representations l_0+n, $n=0,\ldots,l_1-l_0$ appear at least once in the decomposition.) To construct the matrix elements of F_+, F_-, and F_3 in this case we rewrite Eqs. (2.4)–(2.6) in block matrix form:

$$F_3=\begin{bmatrix} N_{l_0,l_0}\times H_3(l_0), & N_{l_0,l_0+1}\times D(l_0), & 0, & \cdots \\ N_{l_0+1,l}\times D(l_0), & N_{l_0+1,l_0+1}\times H_3(l_0+1), & N_{l_0+1,l_0+2}\times D(l_0+1), & 0\cdots \\ 0, & N_{l_0+2,l_0+1}\times D(l_0+1), & N_{l_0+2,l_0+2}\times H_3(l_0+2), & 0\cdots \\ & \cdots & & \end{bmatrix}, \tag{2.17}$$

where the N_{l_i,l_j} are matrices of dimension $n_i\times n_j$ and

$$[D(l)]_{mm'}=\delta_{mm'}\sqrt{(l+1)^2-m^2}. \tag{2.18}$$

Similar expressions can be written for F_+, F_-. The CR (1.4) now reduce to constraints on the matrices $N_{l'_i,l_j}$ in the form

$$N_{l_0,l_0}=N_{l_0,l_0+1}N_{l_0+1,l_0}=N_{l_0,l_0}N_{l_0,l_0+1}=\cdots=0, \tag{2.19}$$

which is, in general, a redundant system of equation for the matrix elements of these matrices.

A particularly interesting case is obtained when the multiplicity of each l in the representation is the same, i.e., $n_i=n$, $i=0,\ldots,l_1-l_0$. In this "degenerate" case all the equations of (2.19) can be satisfied if we choose

$$N_{l,l}=N_{l,l\pm1}=M,$$

where $M^2=0$.

III. INVARIANT EQUATIONS

The study of E(3) invariant equations was initiated by Levi-Leblond[6] who constructed by *ad hoc* methods a nonrelativistic analog of the Dirac equation and studied its properties. In this section, however, we study the construction of such equations from a covariant point of view[7] and especially consider the uniqueness of the nonrelativistic analog of the Dirac equation.

Definition 1: Let an operator realization of p_λ be given (see the Appendix). We say that the equation

$$(L_\lambda p^\lambda+\tilde{m})\psi=0, \quad \psi\in\mathbb{R}^n \tag{3.1}$$

is invariant with respect to E(3) if $L_\lambda p^\lambda$ is a scalar of the E(3) algebra, viz.,

$$[L_\lambda p^\lambda, J_{\mu\nu}]=0. \tag{3.2}$$

We observe that this definition is equivalent to the one introduced in Ref. 4 from a group theoretical point of view for the Lorentz group.

At this point on objection might be raised to the effect that m appears in (3.1) twice, once as a scalar and once as an operator (albeit as a scalar multiplication operator). The answer to this is that this dichotomy is inherent to the definition of mass in nonrelativistic mechanics. In fact m appears as a scalar of the (pure) Galileo group and then is added to the group as an operator through a central extension.[6] In any event since m is constant both as a scalar and as an operator the equations under consideration describe entities with constant mass. Furthermore, by imposing proper constraints on L^μ one can insure (see Proposition 3) that each component of ψ satisfies the Galilean energy-momentum relation. Thus it is appropriate to refer to equations of the form (3.1) as nonrelativistic invariant wave equations.

Corollary 7: Equation (3.1) is invariant with respect to E(3) if and only if

$$[L_\lambda, J_{\mu\nu}]=i[g_{\lambda\mu}L_\lambda-g_{\lambda\nu}L_\mu]. \tag{3.3}$$

Proof: From (3.2) we infer

$$\begin{aligned} 0&=[L^\lambda p_\lambda, J_{\mu\nu}]=L^\lambda[p_\lambda, J_{\mu\nu}]+[L_\lambda, J_{\mu\nu}]p^\lambda \\ &=iL^\lambda[g_{\lambda\mu}p_\nu-g_{\lambda\nu}p_\mu]+[L_\lambda, J_{\lambda\nu}]p^\lambda \\ &=i[g_{\nu\lambda}L_\mu-g_{\mu\lambda}L_\nu]p^\lambda+[L_\lambda, J_{\mu\nu}]p^\lambda, \end{aligned}$$

from which Eq. (3.3) follows.

Furthermore, to insure the physical meaning of such an invariant equation we require that each component of ψ satisfies the Galilean energy-momentum relation

$$E=m+p^2/2m, \tag{3.4}$$

which leads to the following result.

Proposition 3: Each component of ψ satisfies Eq. (3.4) if

$$\{L_\mu, L_\nu\}=L_\mu L_\nu+L_\nu L_\mu=2g_{\mu\nu}I. \tag{3.5}$$

Proof: This result is obvious if we multiply (3.1) by $(L^\mu p_\mu-\tilde{m})$ and require that (3.4) is satisfied. Observe, however, that since $g_{\mu\nu}$ is not diagonal Eq. (3.5) implies

$$L_4^2=0, \quad \{L_4, L_5\}=2I. \tag{3.6}$$

We now turn our attention to finite-dimensional equations which describe nonrelativistic particles with definite spin, viz., equations based on finite-dimensional indecomposable representations of the form given by Eqs. (2.13), (2.14), and (2.16).

To begin with we infer from (3.3) that

$$[[L_3, H_+], H_-]=2L_3. \tag{3.7}$$

Hence using the results in Ref. 4 regarding O(3) invariant equations we obtain

$$L_3=i\cdot D\times\tilde{J}_3(l) \tag{3.8}$$

and consequently

$$L_1=i\cdot D\times\tilde{J}_1(l), \quad L_2=i\cdot D\times\tilde{J}_2(l). \tag{3.9}$$

Furthermore, if we write L_4, L_5 in block form then the CR's

$$[L_4, \tilde{J}_i]=[L_5, \tilde{J}_i]=0 \tag{3.10}$$

imply, using Schur's lemma, that

$$L_4=\lambda_4\times I, \quad L_5=\lambda_5\times I, \tag{3.11}$$

where D, λ_4, λ_5 are $n\times n$ matrices. From Eq. (3.5) it then follows that

$$\{\lambda_4, \lambda_5\}=I, \quad \lambda_5^2=-I, \quad D^2\times\tilde{J}_i^2(l)=I\times I, \tag{3.12}$$

$$\lambda_4^2=\{\lambda_4, D\}=\{\lambda_5, D\}=0.$$

Thus to complete the construction of the invariant equations under consideration we must solve for D, λ_4, λ_5 using the remaining CR. However, from

$$[L_4, J_{34}]=0, \quad [L_5, J_{34}]=-iL_3, \tag{3.13}$$

$$[L_3, J_{34}]=-iL_4, \tag{3.14}$$

$$[[L_5, F_+], F_-] = -2L_4, \tag{3.15}$$

it follows that

$$\lambda_4 N - N\lambda_4 = 0, \tag{3.16}$$

$$\lambda_5 N - N\lambda_5 = D, \tag{3.17}$$

$$(ND - DN) \times \tilde{J}_3^2(l) = \lambda_4, \tag{3.18}$$

and

$$N\lambda_5 N \times \{H_+(l), \quad H_-(l)\} = 2\lambda_4 \times I. \tag{3.19}$$

(The remaining CR lead to the same constraints on λ_4, λ_5, D.)

Proposition 4: Invariant equations of the form (3.1) based on the indecomposable representations (2.13) and (2.14) can be constructed only for $l = \frac{1}{2}$.

Proof: From Eqs. (3.18) and (3.19) it follows that to construct E(3) invariant equations we must have

$$\{H_+(l), H_-(l)\} = \alpha I, \quad \alpha, \beta \in R,$$

and

$$\tilde{J}_3^2 = \beta I. \tag{3.20}$$

However, this can be satisified only for $l = \frac{1}{2}$, where

$$\{H_+[\tfrac{1}{2}], H_-[\tfrac{1}{2}]\} = I, \quad \tilde{J}_3^2 = \tfrac{1}{4} I. \tag{3.21}$$

We conclude from this proposition that invariant equations describing particles with spin $\neq \frac{1}{2}$ must be based on "mixed" indecomposable representations ($l \neq$ const) and will contain, therefore, some extraneous components that must be eliminated by some subsidiary conditions (this is similar to the situation in relativistic mechanics).

Corollary: For $l = \frac{1}{2}$,

$$N\lambda_5 N = 2\lambda_4, \quad [N, D] = 4\lambda_4, \quad D^2 = 4I. \tag{3.22}$$

This is a direct consequence of (3.12), (3.18), (3.19), (3.21).

The nonrelativistic analog to the Dirac equation derived in Refs. 1 and 6 is based on a representation of E(3) in the form (2.13)–(2.15) with dim $N = 2$. These equations are[6]

$$(\boldsymbol{\sigma} \cdot P)\varphi + 2m\chi = 0, \quad (\boldsymbol{\sigma} \cdot \mathbf{P})\chi + E\varphi = 0, \tag{3.23}$$

where φ, χ are two component functions and $\boldsymbol{\sigma}$ are Pauli matrices. We observe however that in these equations φ, χ satisfy the energy-momentum relation in the form $E = P^2/2m$ rather than Eq. (3.4). Hence E should be replaced by $E - m$ to conform to our notation. Using this observation we can rewrite Eq. (3.23) in matrix form as

$$\left\{(I \times \boldsymbol{\sigma}) \cdot \mathbf{P} + \left[\begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} \times I\right] E + m \begin{bmatrix} 0 & 2 \\ -1 & 0 \end{bmatrix} \times I\right\} \begin{bmatrix} \varphi \\ \chi \end{bmatrix} = 0. \tag{3.24}$$

On the other hand, if we use Eqs. (3.12), (3.16)–(3.19), and (3.22) to determine a solution for D, λ_4, λ_5 based on the same representation of E(3), we find

$$\lambda_4 = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}, \quad \lambda_5 = \begin{bmatrix} a & 2 \\ c & -a \end{bmatrix}, \quad D = \begin{bmatrix} 2 & 0 \\ \gamma & -2 \end{bmatrix} \tag{3.25}$$

subject to the constraints

$$a^2 + 2c = -1, \quad 2a + \gamma = 0. \tag{3.26}$$

In matrix form the corresponding equations can be written as

$$\left\{\left(iD \times \frac{\sigma_i}{2}\right) p^i + [\lambda_4 \times I]\tilde{E} + [(\lambda_5 + I) \times I]\tilde{m}\right\} \begin{bmatrix} \varphi \\ \chi \end{bmatrix} = 0, \tag{3.27}$$

and it is easily verified that (3.27) is not equivalent to (3.24).

Furthermore, one can find solutions to Eqs. (3.12) and (3.16)–(3.19) based on higher-dimensional representations of E(3) as illustrated by the following proposition.

Proposition 5: Let N be a 4×4 matrix in the form (2.16) with $\epsilon = \alpha_2 = \alpha_3 = \beta_2 = -\beta_3 = 2$, then the matrices $\lambda_4 = N$ and

$$\lambda_5 = \begin{bmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ \alpha & 1 & 0 & -1 \\ -1 & \alpha & 1 & 0 \end{bmatrix}, \qquad D = 2\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & -2 & 1 & 0 \\ 2+2\alpha & 0 & 0 & -1 \end{bmatrix}, \tag{3.28}$$

where α is an arbitrary parameter, are solutions of equations (3.12) and (3.16)–(3.19).

Thus we showed the existence of a new nonrelativistic analog to the Dirac equation and demonstrated that the number of components in such an equation is indeterminate from a purely nonrelativistic point of view.

We now turn to an attempt to construct a nonrelativistic analog to the Majorana equation based on the self-coupling of a ladder representation l_0, $l_0 + 1$,... (case 1 of Sec. II).

To begin with we introduce an orthogonal basis $\xi_{l,m}$ on the representation space and set

$$L_4 \xi_{l,m} = \sum D_{l,m;l',m'} \xi_{l',m'}. \tag{3.29}$$

However, since $[L_4, J_{\mu\nu}] = 0$ and the representation is irreducible it follows from Schur's lemma that

$$D_{l,m;l',m'} = \rho \delta_{ll'} \delta_{mm'}. \tag{3.30}$$

To calculate the other matrices L_μ we observe that it is sufficient to find L_5. Setting

$$L_5 \xi_{l,m} = \sum c_{l,m;l',m'} \xi_{l',m'} \tag{3.31}$$

we infer from $[L_5, H_3] = 0$ that

$$c_{l,m;l'm'} = c_{l,l',m} \delta_{mm'}. \tag{3.32}$$

Furthermore, from $[L_5, H_\pm] = 0$ we deduce that

$$\alpha_{l,m+1} c_{l,l',m+1} - \alpha_{l',m+1} c_{l,l',m} = 0, \tag{3.33}$$

$$\alpha_{l,m} c_{l,l',m-1} - \alpha_{l',m} c_{l,l',m} = 0. \tag{3.34}$$

By simple algebraic manipulations it then follows that

$$c_{l,m;l',m'} = c_l \delta_{ll'} \delta_{mm'}. \tag{3.35}$$

To compute the c_l's and ρ we now invoke the relation (3.15). By applying this relation to $\xi_{l,m}$ we obtain after a long alge-

bra that $\rho = 0$ and $c_l = c = \text{const}$, viz., $L_4 = 0$, $L_5 = cI$. Using the CR

$$[L_5, J_{i4}] = -iL_i \tag{3.36}$$

this implies that $L_i = 0$. We conclude then that the relativistic Majorana equation has no nonrelativistic analog.

APPENDIX: COMMUTATION RELATIONS FOR E(3)

In this appendix we describe the relationship between the different notations for the generators of the Lie algebra of the Galilean group G and its E(3) subgroup. We also give an explicit differential realization for the commutation relations (CR) of the extended (physical) Galilean group.[6]

1. Real basis[1,6]

The Lie algebra of the (pure) Galilean group has ten generators which we denote by J_i, K_i, P_i, $i = 1, 2, 3$, and E. The J_i's are the generators of the Lie algebras of O(3) the K_i's are the boost generators, and P_i, E are the generators for the translations in space and time, respectively [E(3) is generated by J_i, k_i, $i = 1, 2, 3$].

The nonzero CR of G are

$$\begin{aligned} &[J_i, J_j] = \epsilon_{ijk} J_k, \quad [J_i, K_j] = \epsilon_{ijk} K_k, \\ &[J_i, P_j] = \epsilon_{ijk} P_k, \quad [K_i, E] = P_i. \end{aligned} \tag{A1}$$

The CR for the extended ("physical") Lie algebras of G (which is obtained by a central extension) are the same as in (A1) except that

$$[K_i, P_j] = 0$$

is replaced by

$$[K_i, P_j] = m\delta_{ij}. \tag{A2}$$

Thus the extended group has an additional generator m. However, m is a scalar of the algebra as it commutes with all other generators of G.

2. Complex basis

If we consider G over the complex numbers and define

$$\begin{aligned} &\tilde{J}_j = iJ_j, \quad \tilde{K}_j = iK_j, \quad iP_j, \quad \tilde{E} = iE, \\ &j = 1,2,3, \quad \tilde{m} = im, \end{aligned} \tag{A3}$$

then the CR of G (extended) take the form

$$\begin{aligned} &[\tilde{J}_i, \tilde{J}_j] = i\epsilon_{ijk} \tilde{J}_k, \quad [\tilde{J}_i, \tilde{K}_j] = i\epsilon_{ijk} \tilde{K}_k, \\ &[\tilde{J}_i, \tilde{P}_j] = i\epsilon_{ijk} P_k, \quad [\tilde{K}_i, \tilde{E}] = iP_i, \quad [\tilde{K}_i, \tilde{P}_i] = i\tilde{m}\delta_{ij}. \end{aligned} \tag{A4}$$

3. Covariant notation[7-11]

By introducing the nonsingular "metric"

$$g_{\alpha\beta} = \begin{bmatrix} -I & & 0 \\ & 0 \quad 1 & \\ 0 & & \\ & 1 \quad -1 & \end{bmatrix}, \tag{A5}$$

where I is the unit matrix in three dimensions and

$$\begin{aligned} &J_{ij} = \epsilon_{ijk} \tilde{J}_k, \quad J_{i4} = \tilde{K}_i, \\ &p_i = \tilde{P}_i, \quad p_4 = \tilde{m}, \quad p_5 = \tilde{E} - \tilde{m}, \end{aligned} \tag{A6}$$

we can write the CR of the extended G in covariant notation

$$[J_{\mu\nu}, J_{\rho\sigma}] = i[g_{\nu\rho} J_{\mu\sigma} - g_{\mu\rho} J_{\nu\sigma} + g_{\mu\sigma} J_{\nu\rho} - g_{\nu\sigma} J_{\mu\rho}], \tag{A7}$$

$$[p_\mu, J_{\rho\sigma}] = i[g_{\mu\rho} p_\sigma - g_{\mu\sigma} p_\rho] \tag{A8}$$

(note that $g_{44} = 0$). We observe that the metric tensor $g_{\alpha\beta}$ can be used only to raise and lower indices of vectors over E(3) (Ref. 11), e.g., if $p_{\alpha'} = [p_1, p_2, p_3, \tilde{m}, \tilde{E} - \tilde{m}]$ then

$$p^\alpha = (-p_1, -p_2, -p_3, \tilde{E}, \tilde{m}). \tag{A9}$$

Furthermore, $p_\alpha p^\alpha = \tilde{m}^2$ is the Galilean energy-momentum-mass relation.

A differential realization of the generators (A6) and their CR is given by

$$\begin{aligned} &J_{ij} = i\left[x_j \frac{\partial}{\partial x_i} - x_i \frac{\partial}{\partial x_j}\right], \quad J_{i4} = i\left[t \frac{\partial}{\partial x_i} + m x_i\right], \\ &p_i = -i \frac{\partial}{\partial x_i}, \quad p_4 = im, \quad p_5 = i\left[\frac{\partial}{\partial t} - m\right]. \end{aligned} \tag{A10}$$

4. A basis of raising and lowering operators

Since E(3) and the Lorentz group O(3,1) have the same number of generators (and six of the nine CR are the same) it is convenient to introduce a basis of E(3) similar to the one used by Gel'fand *et al.*[4] to construct the representations and invariant equations of O(3,1). Thus in Gel'fand's notation

$$A_{12} = J_1, \quad A_{13} = J_2, \quad A_{23} = J_1, \quad B_i = K_i, \quad i = 1,2,3. \tag{A11}$$

Hence

$$\begin{aligned} &H_+ = \tilde{J}_1 + i\tilde{J}_2, \quad H_- = \tilde{J}_1 - i\tilde{J}_2, \quad H_3 = \tilde{J}_3, \\ &F_+ = \tilde{K}_1 + i\tilde{K}_2, \quad F_- = \tilde{K}_1 - i\tilde{K}_2, \quad F_3 = \tilde{K}_3. \end{aligned} \tag{A12}$$

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Weight-2 zeros of 3j coefficients and the Pell equation

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All weight-2 zeros of the Wigner 3j coefficients may be obtained from the quadratic Diophantine equation known as Pell's equation. These zeros may then be classified by the orbits of a discrete, infinite-order subgroup of the Lorentz group SO(1,1). This is carried out by transforming the "polynomial part" of a weight-2 3j coefficient to Pellian form and obtaining the fundamental zeros numerically. The relation of this polynomial to a family of binary quadratic forms is also given, together with a discussion of the invariance group.

I. INTRODUCTION AND RÉSUMÉ

A number of papers[1–12] have appeared recently on the subject of (nontrivial) zeros of the angular momentum coefficients known as 3j and 6j symbols. All such zeros are integer solutions of known polynomial expressions,[12,13] that is, of Diophantine equations. The approach to the "zeros problem" via the study of Diophantine equations,[3,5,7–9,11,12] using number theoretic methods, is to be distinguished from the mathematical structure that Racah[14] used to "explain" the first known such zero, which was a Lie algebra–subalgebra relation. Racah's method was extended by Judd,[15] and more recently has been studied systematically (though not exhaustively) by Vanden Berghe *et al.*[16] Other important approaches have been either purely computational,[2,17,18] or through the use of physical models,[13,15,19] or simply suggestive of an underlying structure, not fully implemented.[1,4,6]

The Diophantine approach shows that the number of zeros of the angular momentum coefficients is (denumerably) infinite, but does not suggest physical applications. Although several consequences of the existence of these zeros are known,[13,15,19,20] there is at present no systematic study of the subject. The mathematical relationship—if one exists—between solutions of Diophantine equations and Lie algebra–subalgebra structures has not been established.

The zeros of the 3j and 6j coefficients may all be classified by their weight, which is defined to be the smallest integer in the associated Regge[21] and Bargmann[22] arrays, respectively. The weight may assume values 1,2,... and is related to the total degree of the polynomial (in several variables) whose zeros are sought. The simplest case is weight 1. All weight-1 zeros of both the 3j and 6j coefficients have been given explicitly.[2,5,7–10] Certain general classes of zeros of weight-2 6j coefficients have also been found,[12] but this problem is not completely solved. The success in finding these special zeros may be attributed to the fact that they can be related to the solutions of classic (well-known) Diophantine equations. It appears likely that other Diophantine equations will need to be studied in classifying zeros of higher weight.[11]

In this paper, we classify all zeros of weight-2 3j coefficients in terms of the classic Diophantine equation known as the (generalized) Pell equation. We use a technique developed earlier[12] for weight-2 zeros of 6j coefficients, as described in Secs. II–V. [It is also of interest to study the polynomial in question from a more general viewpoint. This is done in Sec. VI, where it is shown that either the Lorentz group SO(1,1) or the rotation group SO(2) is an underlying symmetry of this polynomial.]

Before giving a more detailed description of the problem, we define some notations used throughout. The real line is denoted by $\mathbb{R}$, the plane by $\mathbb{R}^2$, etc. The set of all integers is denoted by $\mathbb{Z}$, the subset of natural numbers (including zero) by $\mathbb{N}$, and the subset of positive and negative integers by $\mathbb{Z}_+$ and $\mathbb{Z}_-$, respectively. The obvious extensions $\mathbb{Z}^2$, $\mathbb{N}^2$,... are also used. For typographical convenience, we employ one nonstandard notation. We denote the $(n+1)\times(n+1)$ matrix transformation A of a column vector $\mathbf{x}=\mathrm{col}(x_1,x_2,...,x_n,1)$, to a column vector $\mathbf{x}'=\mathrm{col}(x_1',x_2',...,x_n',1)$, where A has the $(n+1)$st row $(0,0,...,0,1)$ by

$$(x_1',...,x_n')=A\cdot(x_1,...,x_n). \tag{1.1}$$

The general polynomial, the set of whose zeros contains all nontrivial zeros of the 3j coefficients, has been given earlier.[12] It was also pointed out that the weight-2 zeros originate from a family of Pell equations. Since the background of this method has been presented in detail in Ref. 12, we proceed immediately to the description of the polynomial whose zeros are the weight-2 zeros of the 3j coefficients. It is convenient to use the variables (u_1,u_2,x_1,x_2) given by the following Regge array:

$$\begin{bmatrix} 2 & x_1 & x_2+u_1-2 \\ u_1+u_2-2 & x_2 & x_1-u_2+2 \\ x_1+x_2-u_2 & u_1 & u_2 \end{bmatrix}. \tag{1.2}$$

The domain $\mathbb{D}^4$ of the variables (u_1,u_2,x_1,x_2) is, by definition, the set of all points $(u_1,u_2,x_1,x_2)\in\mathbb{N}^4$ such that the remaining four entries in the Regge array also belong to $\mathbb{N}$. The polynomial of interest associated with the Regge array (1.2) is given by

$$\begin{aligned} Q_{u_1,u_2}(x_1,x_2) &= 2u_1(u_1-1)(x_1-u_2+1)(x_1-u_2+2) \\ &\quad -4u_1u_2(x_1-u_2+2)x_2 \\ &\quad +2u_2(u_2-1)x_2(x_2-1). \end{aligned} \tag{1.3}$$

The zeros of the Diophantine equation

$$Q_{u_1,u_2}(x_1,x_2)=0 \tag{1.4a}$$

with

$$(u_1,u_2,x_1,x_2)\in\mathbb{D}^4, \tag{1.4b}$$

give all nontrivial zeros for which 2 occurs in the Regge array—a zero of a weight-2 $3j$ coefficient, or, briefly, a weight-2 zero. If any of the entries in the Regge array (1.2) are equal to 1, the polynomial (1.3) reduces to that for special weight-1 zeros. Since *all* weight-1 zeros have already been determined, we will generally restrict the determination of the zeros of $Q_{u_1,u_2}(x_1,x_2)$ to those that satisfy not only

$$(u_1,u_2,x_1,x_2)\in\mathbb{N}^4, \tag{1.5a}$$

but also

$$u_1\geqslant 2,\quad u_2\geqslant 2,\quad x_1\geqslant u_2,\quad x_2\geqslant 2. \tag{1.5b}$$

For completeness, we write down the complete expression for the $3j$ coefficient corresponding to the Regge array (1.2) in the form containing the polynomial (1.3) as a factor:

$$\begin{bmatrix} 2 & x_1 & x_2+u_1-2 \\ u_1+u_2-2 & x_2 & x_1-u_2+2 \\ x_1+x_2-u_2 & u_1 & u_2 \end{bmatrix} = \begin{pmatrix} (u_1+u_2)/2 & (x_1+x_2)/2 & (x_1+x_2+u_1-u_2) \\ (u_1+u_2-4)/2 & (-x_1+x_2)/2 & (x_1-x_2-u_1-u_2+4)/2 \end{pmatrix}$$
$$= (-1)^{x_1+u_1+u_2}\frac{1}{4}\left[\frac{2(u_1+u_2-2)!}{u_1!u_2!}\right]^{1/2}$$
$$\times\left[\frac{(x_1-u_2+3)_{u_2-2}(x_2+1)_{u_1-2}}{(x_1+x_2-u_2+1)_{u_1+u_2+1}}\right]^{1/2} Q_{u_1,u_2}(x_1,x_2), \tag{1.6}$$

where $u_1\geqslant 2$ and $u_2\geqslant 2$ and $(x)_a = x(x+1)\cdots(x+a-1)$ for $a\in\mathbb{N}$ with $(x)_0 = 1$. The $3j$ symbol in this result is related to the standard angular momentum notation by

$$\begin{pmatrix} j_1 & j_2 & j_3 \\ m_1 & m_2 & m_3 \end{pmatrix}.$$

We regard u_1 and u_2 as parameters, and (x_1,x_2) as variables in the expression (1.3); that is, we select values u_1 and u_2 in the domain (1.5) and determine the values of (x_1,x_2) in this domain that are zeros of $Q_{u_1,u_2}(x_1,x_2)$. Observe that each Q_{u_1,u_2} is an inhomogeneous quadratic polynomial in (x_1,x_2). This viewpoint corresponds to interpreting a $3j$ coefficient in terms of a *Wigner operator* specified by the parameters (u_1,u_2) acting in a separable Hilbert space with a standard orthonormal basis given by

$$\{|\tfrac{1}{2}(x_1+x_2),\tfrac{1}{2}(-x_1+x_2)\rangle\,|\,x_1,x_2\in\mathbb{N}\}. \tag{1.7}$$

This operator structure of the $3j$ coefficients has been developed in detail in Ref. 13. We will not pursue it here except to note that the zeros (x_1,x_2) of $Q_{u_1,u_2}(x_1,x_2)$ correspond to vectors in the null space of the Wigner operator specified by (u_1,u_2). These null space vectors are distinct from those belonging to the *characteristic* null space (see Ref. 13). As will be shown in the sequel, for each pair (u_1,u_2) (i.e., a specified Wigner operator), there is a denumerably infinite set of zeros $(x_1,x_2)\in\mathbb{N}^2$ of the quadratic polynomial Q_{u_1,u_2} (hence an infinite set of vectors in the null space of the corresponding Wigner operator). This corresponds to the *hyperbolic structure* of Q_{u_1,u_2} for each pair of parameters (u_1,u_2), as shown in Sec. II.

The "hyperbolic" classification (to be demonstrated) of $3j$ coefficients using the solutions of the Diophantine equation (1.4a) for each pair $(u_1,u_2)\in\mathbb{N}^2$ is not the only one. It must also be possible to classify these zeros by dividing them into finite sets according to the value of the "magic square" parameter of a Regge array. This parameter is the common sum of the entries in the separate rows and columns. It is given by $x_1+x_2+u_1$ for the array (1.2). This suggests a change of coordinates.

Consider the transformation of coordinates

$$(u_1,u_2,x_1,x_2)\mapsto(v_1,v_2,y_1,y_2), \tag{1.8}$$

$$y_1 = u_1,\quad y_2 = x_1-u_2+2,$$
$$v_1 = u_1+u_2-2,\quad v_2 = x_1+x_2-u_2 \tag{1.9a}$$

with the inverse

$$x_1 = -y_1+y_2+v_1,\quad x_2 = -y_2+v_2+2,$$
$$u_1 = y_1,\quad u_2 = v_1-y_1+2. \tag{1.9b}$$

In the new coordinates, the Regge array (1.2) becomes

$$\begin{bmatrix} 2 & y_2-y_1+v_1 & y_1-y_2+v_2 \\ v_1 & v_2-y_2+2 & y_2 \\ v_2 & y_1 & v_1-y_1+2 \end{bmatrix} \tag{1.10a}$$

which has magic square parameter

$$v_1+v_2+2. \tag{1.10b}$$

The domain $\overline{\mathbb{D}}^4$ of the variables (v_1,v_2,y_1,y_2) is defined with the same phrases (*mutatis mutandis*) used in defining the domains $\mathbb{D}^4$ of (u_1,u_2,x_1,x_2), namely, it is the set of all $(v_1,v_2,y_1,y_2)\in\mathbb{N}^4$ with the additional property that the remaining four entries in the Regge array (1.10a) also belong to $\mathbb{N}$. The polynomial (1.3) is expressed in terms of the new variables by

$$Q_{u_1,u_2}(x_1,x_2) = P_{v_1,v_2}(y_1,y_2)$$
$$= 2y_1(y_1-1)y_2(y_2-1)$$
$$-4y_1(v_1-y_1+2)y_2(v_2-y_2+2)$$
$$+2(v_1-y_1+1)(v_1-y_1+2)$$
$$\times(v_2-y_2+1)(v_2-y_2+2). \tag{1.11}$$

The coefficients of $y_1^2y_2^2, y_1^2y_2$, and $y_1y_2^2$ in $P_{v_1,v_2}(y_1,y_2)$ vanish identically in (v_1,v_2). Thus $P_{v_1,v_2}(y_1,y_2)$ is an inhomogeneous quadratic polynomial in (y_1,y_2). This polynomial can have only the finite number of zeros that correspond to zeros of the $3j$ coefficient

$$\begin{pmatrix}(v_1+2)/2 & (-y_1+v_1+v_2+2)/2 & (y_1+y_2)/2\\ (v_1-2)/2 & (y_1-2y_2-v_1+v_2+2)/2 & (-y_1+2y_2-v_2)/2\end{pmatrix}. \tag{1.12}$$

The reason is that for $(v_1,v_2)\in\mathbb{N}^2$, we have $(v_1,v_2,y_1,y_2)\in\overline{\mathbb{D}}^4$ if an only if $(y_1,y_2)\in\mathbb{N}^2$ and

$$0\leqslant y_1\leqslant v_1+2,\quad 0\leqslant y_2\leqslant v_2+2. \tag{1.13}$$

Indeed, as we show in Sec. II, the number of zeros $(y_1,y_2)\in\mathbb{N}^2$ of the Diophantine equation

$$P_{v_1,v_2}(y_1,y_2)=0 \tag{1.14}$$

for given $(v_1,v_2)\in\mathbb{N}^2$ is finite in consequence of its *elliptical structure*.

The set of all $3j$ coefficients is mapped into itself, up to phase, under the group of transformations of the angular momentum quantum numbers $(j_1,m_1,j_2,m_2,j_3,m_3)$ corresponding to permutations of rows, permutations of columns, and transposition of the Regge array. This is a 72-element group which is isomorphic to the direct product group $S_3\times S_3\times S_2$, where S_n denotes the symmetric group on n symbols. Thus each zero of the Diophantine equation (1.4) gives rise to 72 zeros (or less, if the Regge array is symmetric or has some equal columns or rows) corresponding to the permutations and the transposition mentioned above.

We have already used the Regge symmetry to write the entry 2 in the upper left-hand corner of the arrays (1.2) and (1.10a). The 2 remains in this position under an eight element group of transformations K of the variables (u_1,u_2,x_1,x_2) generated by the interchange of columns 2 and 3, of rows 2 and 3, and by transposition (isomorphic to $S_2\times S_2\times S_2$). The transformation group is given explicitly by

$$K=\{I,r,t,rt,tr,trt,rtr,(rt)^2=(tr)^2\}. \tag{1.15a}$$

The matrices r and t, which correspond to column 2–column 3 interchange and transposition, are defined by the matrices

$$r=\begin{pmatrix}0&1&0&0&0\\1&0&0&0&0\\1&0&0&1&-2\\0&-1&1&0&2\\0&0&0&0&1\end{pmatrix},\qquad t=\begin{pmatrix}0&-1&1&0&2\\0&1&0&0&0\\1&1&0&0&-2\\0&0&0&1&0\\0&0&0&0&1\end{pmatrix}. \tag{1.15b}$$

The transformations of (u_1,u_2,x_1,x_2) are then

$$(u_1,u_2,x_1,x_2)\mapsto(u_1',u_2',x_1',x_2')=k\cdot(u_1,u_2,x_1,x_2),\quad k\in K. \tag{1.15c}$$

The Regge symmetries of the $3j$ coefficients imply that the polynomial $Q_{u_1,u_2}(x_1,x_2)$ is invariant under the group K; that is,

$$Q_{u_1',u_2'}(x_1',x_2')=Q_{u_1,u_2}(x_1,x_2), \tag{1.16}$$

for each transformation (1.15c). We do not take the symmetry (1.16) into account in the classification of zeros of $Q_{u_1,u_2}(x_1,x_2)$ given in Sec. V; that is, we have not attempted to partition these zeros into the equivalence classes resulting from the definition $(u_1',u_2',x_1',x_2')\sim(u_1,u_2,x_1,x_2)$, if Eq. (1.16) is satisfied. Thus, with each zero of Eqs. (1.4), we associate a set of 72 zeros, obtained from the given one by the Regge group. Some of these sets will be identical because of (1.16); some elements in a given set may also be equal if the Regge array is symmetric or has equal columns or rows.

Results similar to the above also apply to the polynomial $P_{v_1,v_2}(y_1,y_2)$. [We will not deal directly with this expression, but let us note that its zeros can be obtained from those of $Q_{u_1,u_2}(x_1,x_2)$ by use of the transformation (1.9).]

II. TRANSFORMATION TO DIAGONAL FORM

In studying the properties of the polynomials $Q_{u_1,u_2}(x_1,x_2)$ and $P_{v_1,v_2}(y_1,y_2)$ defined by Eqs. (1.3) and (1.11), respectively, we can regard (u_1,u_2,x_1,x_2) and (v_1,v_2,y_1,y_2) as arbitrary points in $\mathbb{R}^4$. We do this in much of this section, except when we want to relate the results to zeros of $3j$ coefficients.

The inhomogeneous polynomial (1.3) is written in standard matrix form as

$$Q_{u_1,u_2}(x_1,x_2)=(x_1\ x_2\ 1)A\begin{pmatrix}x_1\\x_2\\1\end{pmatrix}. \tag{2.1}$$

where A is the real 3×3 symmetric matrix

$$A=(a_{ij}), \tag{2.2a}$$

with

$$\begin{aligned}&a_{11}=2u_1(u_1-1),\quad a_{12}=-2u_1u_2,\\&a_{22}=2u_2(u_2-1),\quad a_{13}=-u_1(u_1-1)(2u_2-3),\\&a_{23}=2u_1u_2(u_2-2)-u_2(u_2-1),\\&a_{33}=2u_1(u_1-1)(u_2-1)(u_2-2).\end{aligned} \tag{2.2b}$$

The polynomial (2.1), that is, the matrix A, is brought to diagonal form using the upper triangular transformation (see Ref. 12 for the details):

$$\Delta_A=\begin{pmatrix}a_{11}&a_{12}&a_{33}\\0&\alpha_{22}&\alpha_{23}\\0&0&1\end{pmatrix}, \tag{2.3a}$$

where

$$\alpha_{22}=\det\begin{bmatrix}a_{11}&a_{12}\\a_{12}&a_{22}\end{bmatrix},\quad \alpha_{23}=\det\begin{bmatrix}a_{11}&a_{13}\\a_{12}&a_{23}\end{bmatrix}. \tag{2.3b}$$

Defining new variables (ξ_1,ξ_2) by

$$\begin{pmatrix}\xi_1\\\xi_2\\1\end{pmatrix}=\Delta_A\begin{pmatrix}x_1\\x_2\\1\end{pmatrix}, \tag{2.4a}$$

we obtain

$$(\det\Delta_A)Q_{u_1,u_2}(x_1,x_2)=p_2\xi_1^2+\xi_2^2+p_1p_3, \tag{2.4b}$$

where

$$p_1=a_{11},\quad p_2=\alpha_{22},\quad p_3=\det A,\quad \det\Delta_A=p_1p_2. \tag{2.4c}$$

[Note that (2.4b) is a true "quadratic form" with the variable $\xi_3 = 1$.] Explicit evaluation of the p_i and α_{23}, using the coefficients (2.2), gives

$$p_1 = 2u_1(u_1 - 1), \quad p_2 = -4u_1u_2(u_1 + u_2 - 1),$$
$$p_3 = \tfrac{1}{2}(u_1 - 1)(u_2 - 1)(u_1 + u_2)p_2, \tag{2.5}$$
$$\alpha_{23} = \tfrac{1}{2}(u_1 - 1)p_2.$$

Let us digress to consider the application of this diagonalization procedure to the problem of $3j$ coefficients; in this case all the entries in the matrix Δ_A are integral. Accordingly, the map $(x_1,x_2)\mapsto(\xi_1,\xi_2)$ given by Eq. (2.4a) is, for $(x_1,x_2)\in\mathbf{N}^2$, from $\mathbf{N}^2$ to $\mathbf{Z}^2$. The converse of this result is, however, not true in general, since the inverse transformation is

$$x_2 = (\xi_2 - \alpha_{23})/p_2, \tag{2.6a}$$
$$x_1 = (\xi_1 - a_{12}x_2 - a_{13})/p_1. \tag{2.6b}$$

Nonetheless, if solutions of

$$Q_{u_1,u_2}(x_1,x_2) = 0 \tag{2.7a}$$

exist in the domain (1.5), they must correspond to solutions $(\xi_1,\xi_2)\in\mathbf{Z}^2$ of the Diophantine equation

$$p_2\xi_1^2 + \xi_2^2 + p_1p_3 = 0. \tag{2.7b}$$

This equation can be simplified further because the coefficient α_{23} contains p_2 as a factor. Hence we can write

$$\xi_2/p_2 = x_2 + \tfrac{1}{2}(u_1 - 1), \tag{2.8a}$$

so that ξ_2/p_2 is always half-integral for $x_2\in\mathbf{N}$ and $u_1\in\mathbf{N}$. Consequently, it is necessary that ξ_2 have the form

$$\xi_2 = -2u_1u_2(u_1 + u_2 - 1)y, \quad y\in\mathbf{Z}, \tag{2.8b}$$

in order that $x_2\in\mathbf{N}$.

Let us return to the general diagonalization (2.4b) for which the only restriction is $\det\Delta_A \neq 0$, that is, $p_1\neq 0, p_2\neq 0$. Under the further change of variable

$$\xi_1 = x, \quad x\in\mathbf{R}, \tag{2.9a}$$
$$\xi_2 = -2u_1u_2(u_1 + u_2 - 1)y, \quad y\in\mathbf{R}, \tag{2.9b}$$

(2.4b) reduces to

$$2u_1(u_1 - 1)Q_{u_1,u_2}(x_1,x_2)$$
$$= x^2 - u_1u_2(u_1 + u_2 - 1)y^2$$
$$+ u_1(u_1 - 1)^2(u_2 - 1)(u_1 + u_2). \tag{2.10}$$

The relation between the variables (x_1,x_2) and (x,y) is

$$x_1 = \frac{x + u_1u_2y}{2u_1(u_1 - 1)} + \frac{1}{2}(u_2 - 3), \tag{2.11a}$$
$$x_2 = \tfrac{1}{2}(y - u_1 + 1). \tag{2.11b}$$

Relation (2.10) is valid for all points $(u_1,u_2,x_1,x_2)\in\mathbf{R}^4$, excepting the points that have $u_1 = 0$ or $u_1 = 1$, with the transformation between coordinates given by Eqs. (2.11).

The problem of finding all nontrivial weight-2 zeros of $3j$ coefficients has now been reduced to the following: For each pair $(u_1,u_2)\in\mathbf{N}^2$ with $u_1\geqslant 2$ and $u_2\geqslant 2$, find all solutions $(x,y)\in\mathbf{Z}^2$ of the Pell equation

$$x^2 - u_1u_2(u_1 + u_2 - 1)y^2$$
$$= -u_1(u_1 - 1)^2(u_2 - 1)(u_1 + u_2) \tag{2.12}$$

such that the coordinates (x_1,x_2) given by Eqs. (2.11) satisfy $(x_1,x_2)\in\mathbf{N}^2$ and $x_1\geqslant u_2, x_2\geqslant 2$. The corresponding weight-2 $3j$ coefficients that are zero are then given by Eq. (1.6).

That such zeros exist is shown by the example $u_1 = u_2 = 2$, $x = 38$, $y = 11$, $x_1 = 20$, $x_2 = 5$, which corresponds to

$$\begin{pmatrix} 2 & \frac{25}{2} & \frac{25}{2} \\ 0 & -\frac{15}{2} & \frac{15}{2} \end{pmatrix} = 0. \tag{2.13}$$

As will be shown in the next section, this zero is one of a denumerably infinite family corresponding to certain points $(x,y)\in\mathbf{N}^2$ on the hyperbola

$$x^2 - 12y^2 = -8. \tag{2.14}$$

We refer to the classification of the weight-2 zeros of $3j$ coefficients using the Pell equation (2.12) as the *hyperbolic classification*. This method is developed in some detail in Sec. III.

The diagonalization procedure described by Eqs. (2.3)–(2.5) also applies to the polynomial

$$P_{v_1,v_2}(y_1,y_2) = (y_1\ y_2\ 1)B\begin{pmatrix} y_1 \\ y_2 \\ 1 \end{pmatrix}, \tag{2.15}$$

where B is the real 3×3 symmetric matrix

$$B = (b_{ij}), \tag{2.16a}$$

with

$$b_{11} = 2(v_2 + 1)(v_2 + 2), \quad b_{12} = 2(v_1 + 1)(v_2 + 1),$$
$$b_{22} = 2(v_1 + 1)(v_1 + 2),$$
$$b_{13} = -(v_2 + 1)(v_2 + 2)(2v_1 + 3), \tag{2.16b}$$
$$b_{23} = -(v_1 + 1)(v_1 + 2)(2v_2 + 3),$$
$$b_{33} = 2(v_1 + 1)(v_1 + 2)(v_2 + 1)(v_2 + 2).$$

The final result, which is analogous to Eqs. (2.10) and (2.11), is

$$2(v_2 + 1)(v_2 + 2)P_{v_1,v_2}(y_1,y_2)$$
$$= X^2 + (v_1 + 1)(v_2 + 1)(v_1 + v_2 + 3)Y^2$$
$$- (v_1 + 2)(v_2 + 1)(v_2 + 2)^2(v_1 + v_2 + 2), \tag{2.17}$$

where the transformation between the coordinates (y_1,y_2) and (X,Y) is

$$y_1 = \frac{X - (v_1 + 1)(v_2 + 1)Y}{2(v_2 + 1)(v_2 + 2)} + \frac{1}{2}(v_1 + 2), \tag{2.18a}$$
$$y_2 = \tfrac{1}{2}(Y + v_2 + 2). \tag{2.18b}$$

Relation (2.17) is valid for all points $(v_1,v_2,y_1,y_2)\in\mathbf{R}^4$, excepting the points having $v_2 = -2$ or $v_2 = -1$, with the transformation between coordinates given by Eqs. (2.18).

The problem of finding all nontrivial weight-2 zeros of $3j$ coefficients has now been reduced to the following: For each pair $(v_1,v_2)\in\mathbf{N}^2$, with $v_1\geqslant 2$ and $v_2\geqslant 2$, find all solutions $(X,Y)\in\mathbf{Z}^2$ that belong to the ellipse

$$X^2 + (v_1 + 1)(v_2 + 1)(v_1 + v_2 + 3)Y^2$$
$$= (v_1 + 2)(v_2 + 1)(v_2 + 2)^2(v_1 + v_2 + 2) \tag{2.19}$$

such that the coordinates (y_1,y_2) given by Eqs. (2.18) satisfy $(y_1,y_2)\in\mathbf{N}^2$ and $2\leqslant y_1\leqslant v_1$, $2\leqslant y_2\leqslant v_2$. The corresponding

weight-2 $3j$ coefficients that are zero are then given by Eq. (1.12).

That such zeros exist is shown by the example $v_1 = 2$, $v_2 = 23$, $X = 1080$, $Y = 15$, $y_1 = 2$, $y_2 = 20$, which corresponds to the zero given by Eq. (2.13) [see Eqs. (1.9a) and (1.12)]. This zero comes from the ellipse

$$X^2 + 2016Y^2 = 1620\,000. \tag{2.20}$$

We refer to the classification of the weight-2 zeros of $3j$ coefficients using integral points on the ellipse (2.19) as the *elliptical classification*. All weight-2 zeros of $3j$ coefficients can be classified by either the hyperbolic or the elliptic scheme, *or both*.

III. GENERAL PROCEDURE FOR SOLVING PELL'S EQUATION

Our procedure for solving Pell's equation,

$$x^2 - Dy^2 = N, \tag{3.1}$$

where D is a positive integer and N integral but not necessarily positive, has been described in detail in Ref. 12. All proofs of the results stated below are given there. For the reader's convenience, we summarize briefly this *method of orbits*.

We order all points $(x,y)\in\mathbb{R}^2$ by the rule $(x,y) < (x',y')$ if $x < x'$ and $(x,y) < (x,y')$ if $y < y'$. The point (x,y) is called positive if $x > 0$ and $y \geqslant 0$. We also use the following notations.

(i) (u_0,v_0) denotes the least positive solution of

$$u^2 - Dv^2 = 1 \tag{3.2}$$

(such a solution always exists; see, for example, LeVeque[23]).

(ii) (x_0,y_0) denotes the least positive solution of the Pell equation (3.1) for given D and N, whenever solutions of this equation exist.

With the solution (u_0,v_0) of Eq. (3.2) we associate the matrix g_0 of unit determinant given by

$$g_0 = \begin{pmatrix} u_0 & v_0 D \\ v_0 & u_0 \end{pmatrix}. \tag{3.3}$$

The basic result for solutions of the general Pell equation (3.1) is the following: For each $n\in\mathbb{Z}$ and each solution (x,y) of (3.1), the point $(x^{(n)},y^{(n)})$ defined by

$$\begin{pmatrix} x^{(n)} \\ y^{(n)} \end{pmatrix} = g_0^n \begin{pmatrix} x \\ y \end{pmatrix} \tag{3.4}$$

is a solution of (3.1).

Relation (3.4) is the principal result needed for classifying all solutions of Pell's equation (3.1) by means of the orbits of the group G_0 defined by

$$G_0 = \{ g_0^n \,|\, n\in\mathbb{Z}\}. \tag{3.5}$$

Each $g\in G_0$ maps a point $(x,y)\in\mathbb{R}^2$ of the hyperbola $x^2 - Dy^2 = N$ to a new point

$$(x,y) \overset{g}{\mapsto} (x',y') = g(x,y) \tag{3.6a}$$

of the hyperbola. The action of g on the point (x,y) is given by matrix multiplication

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = g \begin{pmatrix} x \\ y \end{pmatrix}. \tag{3.6b}$$

In particular, $(x,y)\in\mathbb{Z}^2$ implies $(x',y')\in\mathbb{Z}^2$, and conversely. The orbit of the point $(x,y)\in\mathbb{Z}^2$ is the set of points $G_0(x,y)$ defined by

$$G_0(x,y) = \{ g(x,y) \,|\, g\in G_0\}. \tag{3.7}$$

A set of *fundamental solutions with respect to* G_0 of Pell's equation (3.1) is given by

$$\mathbb{D} = \{(x,y) \,|\, x^2 - Dy^2 = N;\ (x,y)\in\mathbb{N}^2;\ 1 \leqslant y \leqslant u_0x_0 + v_0y_0 - 1\}. \tag{3.8a}$$

Here (u_0,v_0) and (x_0,y_0) denote the least positive solutions of Eqs. (3.2) and (3.1), respectively. The set $\mathbb{D}$ depends, of course, on D and N in Eq. (3.1), that is, we really have

$$\mathbb{D} = \mathbb{D}(D,N). \tag{3.8b}$$

The set of all integer solutions of the Pell equation (3.1) belonging to the *positive branch* of the hyperbola ($x > 0$, if $N > 0$; $y > 0$, if $N < 0$) is given by the sets

$$g_0^n \mathbb{D}, \quad n = 0, \pm 1, \pm 2, \ldots . \tag{3.9}$$

Here multiplication of $\mathbb{D}$ from the left by g_0^n means that each element of $\mathbb{D}$ is multiplied by g_0^n. Alternatively, the set of all integer solutions (3.9) of Pell's equation belonging to the positive branch may be classified by orbits under the action of the group G_0,

$$G_0(x,y) = \{g_0^n (x,y) \,|\, n = 0, \pm 1, \pm 2, \ldots\}, \tag{3.10a}$$

where

$$(x,y)\in\mathbb{D}. \tag{3.10b}$$

One obtains, of course, *all* integer solutions of Eq. (3.1) from those given by the sets (3.9) [or (3.10)] by adjoining those with reversed sign of the x coordinate if $N > 0$ and of the y coordinate if $N < 0$.

The number of orbits, that is, the number $|\mathbb{D}|$ of elements in the set $\mathbb{D}$, is not known in general. Bounds on this number have been given by Stolt.[24] For the special Pell equation of interest here, we determine the number of orbits numerically, as described in the next section.

IV. PROPERTIES OF THE PELL EQUATION FOR WEIGHT-2 ZEROS OF 3j COEFFICIENTS

The Pell equation of interest here for determining all weight-2 zeros of $3j$ coefficients is given by Eq. (2.12). Because both D and N are polynomials in the variables $(u_1,u_2)\in\mathbb{N}^2$, this Pell equation has many nice properties that allow us to give a reasonably comprehensive treatment. In terms of the notation (3.1) for the general Pell equation, Eq. (2.12) is

$$x^2 - Dy^2 = N, \tag{4.1a}$$

where the integers D and N are given by

$$D = u_1u_2(u_1 + u_2 - 1), \tag{4.1b}$$

$$N = -u_1(u_1 - 1)^2(u_2 - 1)(u_1 + u_2), \tag{4.1c}$$

where

$$(u_1,u_2)\in\mathbb{N}^2, \quad u_1 \geqslant 2, \ u_2 \geqslant 2. \tag{4.1d}$$

Throughout this section, D and N denote the polynomials (4.1b) and (4.1c), respectively, subject to conditions (4.1d) unless otherwise specified.

One of the special properties of Eq. (4.1a) is that it possesses two *parametric solutions*. Namely, for all

$$(u_1,u_2,x,y)\in\mathbb{R}^4, \tag{4.2}$$

the following values of x and y solve Eq. (4.1a):

$$x=u_1(u_1-1),\quad y=u_1-1; \tag{4.3a}$$

$$x=u_1(u_1+2u_2-1),\quad y=u_1+1. \tag{4.3b}$$

For all $(u_1,u_2)\in\mathbb{N}^2$ with $u_1\geqslant 2$ and $u_2\geqslant 2$, one can prove by elementary methods that these two solutions are the only parametric solutions of Eq. (4.1a). In fact, each parametric solution must have $y=u_1+a$, $a\in\mathbb{Z}$, since this is the only way that the term $-u_1^4u_2$ on the right-hand side can be canceled identically by a term from the left-hand side. The values $a=\pm 1$ are then determined by substituting $y=u_1+a$ in Eq. (4.1a).

Numerical calculations show that the parametric solution (4.3a) is sometimes, but not always, the smallest positive solution (x_0,y_0) of the equation. More generally, it can be shown that

$$(u_1-1)\sqrt{(u_2-1)/u_2}<y_0\leqslant u_1-1, \tag{4.4}$$

but we cannot give the exact result for (x_0,y_0).

Let us summarize, for the special Pell equation (4.1), the method of solution given in Sec. III [see Eqs. (3.8)]. The fundamental solutions are

$$\mathbb{D}(u_1,u_2)=\mathbb{D}(D,N), \tag{4.5}$$

where D and N are defined by Eqs. (4.1b) and (4.1c). As noted earlier, (u_0,v_0) and (x_0,y_0) are the least positive solutions, respectively, of $u^2-Dv^2=1$ and $x^2-Dy^2=N$. The set $\mathbb{D}(u_1,u_2)$ contains at least two points, namely, the two parametric solutions (4.3). For a specific (u_1,u_2), the set of all integral solutions of Eq. (4.1a) belonging to the positive branch of the hyperbola is given by

$$g_0^n\mathbb{D}(u_1,u_2),\quad n=0,\pm 1,\pm 2,\ldots. \tag{4.6}$$

The orbit $G_0(x,y)$ of the fundamental solution $(x,y)\in\mathbb{D}(u_1,u_2)$ is

$$G_0(x,y)=\{g_0^n(x,y)\,|\,n\in\mathbb{Z}\}. \tag{4.7}$$

An integral solution of the Pell equation does not, in general, correspond to a zero of the $3j$ coefficient. This is because the map $(x,y)\mapsto(x_1,x_2)$ given by Eqs. (2.11) is not from integers into integers. For that property to hold, it is necessary (but not sufficient) that $u_1(u_1-1)$ divide $x+u_1u_2y$; that is,

$$k=(x+u_1u_2y)/u_1(u_1-1)\in\mathbb{Z}. \tag{4.8}$$

When this condition is fulfilled, the map (2.11) $(x,y)\mapsto(x_1,x_2)$ is

$$x_1=(k+u_2-3)/2, \tag{4.9a}$$

$$x_2=(y-u_1+1)/2. \tag{4.9b}$$

From the above results we conclude the following: For each $(u_1,u_2)\in\mathbb{N}$ with $u_1\geqslant 2$, $u_2\geqslant 2$, the necessary and sufficient conditions that a solution (x,y) of the Pell equation correspond to a weight-2 zero of a $3j$ coefficient are

(i) $x+u_1u_2y=0\ [\mathrm{mod}\ u_1(u_1-1)]$;

(ii) (u_1,u_2) and (k,y) satisfy $k\geqslant u_2+3$ with k and u_2 of opposite parity, and $y\geqslant u_1+3$ with y and u_1 of opposite parity.

We formulate two theorems that are basic for obtaining the zeros of the $3j$ coefficients from the zeros of the Pell equation. First, we define the subset $\mathbb{A}(u_1,u_2)$ of the set $\mathbb{D}(u_1,u_2)$ of fundamental solutions of the Pell equation by

$$\mathbb{A}(u_1,u_2)=\{(x,y)\in\mathbb{D}(u_1,u_2)\,|\,\text{condition (i) holds}\}. \tag{4.10}$$

Theorem 4.1: A necessary and sufficient condition that a solution (x',y') of the Pell equation be divisible by $u_1(u_1-1)$ is that $(x',y')\in G_0(x,y)$, where $(x,y)\in\mathbb{A}(u_1,u_2)$.

Proof: Let (x,y) and (x',y') be *any* two integer solutions of the Pell equation that are related by $(x',y')=g_0(x,y)$, where g_0 is the generator (3.3) of G_0. We prove the theorem by showing that, if $x+u_1u_2y$ is divisible by $u_1(u_1-1)$, then so is $x'+u_1u_2y'$, and conversely. Define k and k' [see (4.8)] by

$$k=(x+u_1u_2y)/u_1(u_1-1), \tag{4.11a}$$

$$k'=(x'+u_1u_2y')/u_1(u_1-1). \tag{4.11b}$$

The transformation $(x,y)\mapsto(x',y')=g_0(x,y)$ then gives $(k,y)\mapsto(k',y')=h_0(k,y)$; that is,

$$\begin{pmatrix}k'\\y'\end{pmatrix}=h_0\begin{pmatrix}k\\y\end{pmatrix}, \tag{4.12a}$$

where h_0 is the matrix of unit determinant defined by

$$h_0=\begin{pmatrix}u_0+u_1u_2v_0 & -u_2(u_2-1)v_0\\ u_1(u_1-1)v_0 & u_0-u_1u_2v_0\end{pmatrix}. \tag{4.12b}$$

Clearly, k and y integral imply k' and y' integral, and conversely, since h_0^{-1} is obtained from h_0 by replacing v_0 by $-v_0$. ■

The significance of Theorem 4.1 is in showing that for obtaining solutions of the Pell equation (4.1a) that map back to integer solutions (x_1,x_2) of $Q_{u_1,u_2}(x_1,x_2)=0$ it is sufficient to consider those fundamental solutions in the set $\mathbb{A}(u_1,u_2)$. We must still select from the orbit $G_0(x,y)$, $(x,y)\in\mathbb{A}(u_1,u_2)$, those points having parity such that (x_1,x_2) defined by Eqs. (4.9) are integral. This selection is also reduced to the set $\mathbb{A}(u_1,u_2)$ by the next result.

Theorem 4.2: Each point in the orbit $G_0(x,y)$, $(x,y)\in\mathbb{A}(u_1,u_2)$ has the same parity as the point (x,y).

Proof: It is sufficient to show that the maps $(x,y)\mapsto(x',y')=g_0(x,y)$ and $(x,y)\mapsto(x'',y'')=g_0^{-1}(x,y)$ conserve the parity of (x,y) for any integer solution of the Pell equation. We do this by considering all cases. To this end we write $(a,b)=(e,o)$ if the integer pair (a,b) has a even and b odd, etc. Then for $(u_1,u_2)=(o,o)$ we have that D is odd, N is even, and $(x,y)=(e,e)$ or (o,o), while $(u_0,v_0)=(o,e)$ or (e,o). For $(u_1,u_2)\neq(o,o)$, we have that D is even, N is even, and $(x,y)=(e,e)$ or (e,o), while $(u_0,v_0)=(o,e)$ or (o,o). Considering all eight cases in turn, we verify parity conservation for the map $(x,y)\mapsto(x',y')=g_0(x,y)$. This result also applies to $(x,y)\mapsto(x'',y'')=g_0^{-1}(x,y)$, since g_0^{-1} is obtained from g_0 by the map $v_0\mapsto -v_0$, which conserves parity. ■

It remains to explain briefly our numerical method for solving the general Pell equation (3.1), where D is a positive, nonsquare integer. We do not treat the elliptical case here, although, in fact, it is much simpler than the hyperbolic case.

If D is a perfect square, there are, as in the elliptical case, only a finite number of solutions for given N, and these are easily dealt with.

Let us choose D and N randomly (in some appropriate fashion) from a very large integer lattice of (D,N) points. Then the Pell equation has, with high probability, no solutions at all. LeVeque[23] gives bounds on x and y [depending on (u_0,v_0), D, and N] such that if the equation has solutions it must have at least one satisfying these bounds. In our case, Eq. (4.1a), there are parametric solutions, so this problem does not arise.

If we take the least positive solution (x_0,y_0) and operate on it as in Eq. (3.4) (with $n=1$) we get the value $(x_0^{(1)},y_0^{(1)})$, the second point on the first orbit. We then solve for all $(x',y') < (x_0^{(1)},y_0^{(1)})$ thus generating the set $\mathbb{D}$ of (3.8a), and hence all fundamental solutions of our special Pell equation. The procedure is to transpose the equation to $x^2 = Dy^2 + N$ and to let y vary from y_0 to $y_0^{(1)}$. For each y, we test the right-hand side of this expression for "squareness"; whenever it is a square, we have a solution. We used various Cray computing machines and worked in double precision. Since Crays have not been designed with such number theoretic problems in mind, it was necessary to do some preprocessing in order to speed up the calculations. Briefly, this consisted in examining a fixed number of trailing bits in $Dy^2 + N$ to eliminate those values which could not possibly be squares. This is quite fast compared to determining whether the expression in question is a square.

There was one further problem of a technical nature. The process described above requires knowledge of the matrix g_0 [Eq. (3.3)], hence of (u_0,v_0), the least positive solution of Eq. (3.2). A look at Kortum and McNiel[25] shows that these integers can be very large indeed; manipulating them would require multiprecision arithmetic, where "multi" means greater than "double." The very large solution appearing in the set $\mathbb{D}$ would probably be of no interest in the physics of the present problem; consequently, we made no effort to calculate all orbits in these cases.

Finally, the code was modified to exclude solutions not satisfying the divisibility conditions of Eq. (4.8); parity violations were dealt with by eye.

V. THE WEIGHT-2 ZEROS OF 3j COEFFICIENTS

We have tabulated in Table I the elements (x,y) in the set $\mathbb{D}(u_1,u_2)$ for $2\leqslant u_1\leqslant 6$, $2\leqslant u_2\leqslant 6$, together with the integer k defined by Eq. (4.8), and the solution (u_0,v_0) of $u^2 - Dv^2 = 1$. These integers are presented as $(x,y)(k)$ when k exists, and as (x,y) otherwise. Recall that $\mathbb{A}(u_1,u_2)$ is the subset of all fundamental solutions of the Pell equation (4.1a) such that $(x,y)\in\mathbb{D}(u_1,u_2)$ and $x + u_1u_2\,y$ is divisible by $u_1(u_1-1)$, this quotient defining the integer k. Thus the coordinates (k,y) and the elements of the matrix h_0 in Eqs. (4.12) are completely determined for each point $(x,y)\in\mathbb{A}(u_1,u_2)$.

We shall now show how to obtain all weight-2 zeros of the $3j$ coefficients from the fundamental solutions $(x,y)\in\mathbb{A}(u_1,u_2)$, Eqs. (4.12), and Eqs. (4.9). We must take into account the transformations (4.8) and (4.9), as well as the parity requirements and conditions $k\geqslant u_2+3$ and $y\geqslant u_1+3$ given just below Eqs. (4.9).

Let L denote the linear transformation

$$\begin{pmatrix} k \\ y \end{pmatrix} = L \begin{pmatrix} x \\ y \end{pmatrix}, \tag{5.1a}$$

$$L = \begin{pmatrix} 1/u_1(u_1-1) & u_1u_2/u_1(u_1-1) \\ 0 & 1 \end{pmatrix}. \tag{5.1b}$$

The group H_0 defined by

$$H_0 = LG_0L^{-1} = \{h_0^n \mid n\in\mathbb{Z}\} \tag{5.2}$$

is isomorphic to G_0. The matrix h_0 [see Eq. (4.12b)] is completely determined by (u_0,v_0) and (u_1,u_2).

Next, we define the set $\mathbb{B}(u_1,u_2)$ to be the image of $\mathbb{A}(u_1,u_2)$ under the transformation L,

$$\mathbb{A}(u_1,u_2) \overset{L}{\mapsto} \mathbb{B}(u_1,u_2). \tag{5.3}$$

Thus the elements of $\mathbb{B}(u_1,u_2)$ are the pairs of integers $(k,y)\in\mathbb{N}^2$ obtained by applying the transformation L to each element $(x,y)\in\mathbb{A}(u_1,u_2)$.

We can now prove the following result.

Theorem 5.1: For each $h\in H_0$, the transformation

$$(k,y)\mapsto h(k,y), \quad (k,y)\in\mathbb{B}(u_1,u_2)$$

conserves parity; that is, the integer pair $(k',y') = h(k,y)$ has the same parity as (k,y).

Proof: It is sufficient to prove that the transformation $(n_1,n_2)\mapsto h_0(n_1,n_2)$ conserves the parity of (n_1,n_2), where (n_1,n_2) is any pair of integers. This is done by considering all cases for (u_1,u_2), (u_0,v_0), and (n_1,n_2). We find that the diagonal elements of the matrix h_0 [see Eq. (4.12b)] are always odd and the off-diagonal ones even. This implies that $(n_1',n_2') = h_0(n_1,n_2)$ and (n_1,n_2) have the same parity. ■

The significance of Theorem 5.1 for weight-2 zeros of $3j$ coefficients is that we can restrict our considerations to those elements $(k,y)\in\mathbb{B}(u_1,u_2)$ that satisfy the required parity properties. This motivates us to define the subset $\mathbb{S}(u_1,u_2)$ of $\mathbb{B}(u_1,u_2)$ by

$$\mathbb{S}(u_1,u_2) = \{(k,y)\in\mathbb{B}(u_1,u_2) \mid u_2 + k \text{ odd};\ u_1 + y \text{ odd}\}. \tag{5.4}$$

Not all points (k,y) in the set $\mathbb{S}(u_1,u_2)$ are mapped by the transformation (4.9) to coordinates (x_1,x_2) that give weight-2 zeros of a $3j$ coefficient. This is because the "threshold conditions" $k\geqslant u_2+3$, $y\geqslant u_1+3$ must still be satisfied. This situation suggests defining the pair of integers $(k^*,y^*)\in\mathbb{N}^2$ to be the least pair in the sets

$$\ldots,h_0^{-2}\mathbb{S}(u_1,u_2),h_0^{-1}\mathbb{S}(u_1,u_2),\mathbb{S}(u_1,u_2),$$
$$h_0\mathbb{S}(u_1,u_2),h_0^2\mathbb{S}(u_1,u_2),\ldots, \tag{5.5a}$$

such that

$$k^*\geqslant u_2+3, \quad y^*\geqslant u_1+3. \tag{5.5b}$$

[Note that h_0 is defined in (4.12b).] We find, in fact, that

$$(k^*,y^*)\in h_0^{-1}\mathbb{S}(u_1,u_2),\ \mathbb{S}(u_1,u_2),\ \text{or}\ h_0\mathbb{S}(u_1,u_2). \tag{5.6}$$

This result may be proved by using the parametric solution (4.3a). This parametric point gives

TABLE I. Fundamental solutions of Pell's equation.

(u_1,u_2)	(u_0,v_0)	$(x,y)(k)$ and (x,y)
(2,2) (two orbits)	(7,2)	(2,1)(3) (10,3)(11)
(2,3) (two orbits)	(5,1)	(2,1)(4) (14,3)(16)
(2,4) (three orbits)	(19,3)	(2,1)(5) (18,3)(21) (82,13)(93)
(2,5) (four orbits)	(31,4)	(2,1)(6) (22,3)(26) (38,5)(44) (178,23)(204)
(2,6) (six orbits)	(55,6)	(2,1)(7) (16,2)(20) (26,3)(31) (82,9)(95) (128,14)(148) (394,43)(455)
(3,2) (two orbits)	(5,1)	(6,2)(3) (18,4)(7)
(3,3) (six orbits)	(161,24)	(6,2)(4) (24,4)(10) (66,10)(26) (174,26)(68) (456,68)(178) (1194,178)(466)
(3,4) (four orbits)	(17,2)	(6,2)(5) (30,4)(13) (66,8)(27) (186,22)(75)
(3,5) (six orbits)	(41,4)	(6,2)(6) (36,4)(16) (69,7)(29) (111,11)(46) (204,20)(84) (594,58)(244)
(3,6) (square)	(1,0)	(6,2)(7) (42,4)(19)
(4,2) (four orbits)	(19,3)	(12,3)(3) (28,5) (68,11)(13) (132,21)(25)
(4,3) (four orbits)	(17,2)	(12,3)(4) (36,5)(8) (108,13)(22) (228,27)(46)
(4,4) (eight orbits)	(127,12)	(12,3)(5) (44,5) (68,7)(15) (156,15)(33) (348,33)(73) (772,73) (1132,107)(237) (2508,237)(525)
(4,5) (ten orbits)	(721,57)	(12,3)(6) (52,5) (108,9)(24) (212,17)(46) (492,39)(106) (948,75)(204) (2188,173) (4212,333)(906) (8108,641)(1744) (18708,1479)(4024)
(4,6) (nine orbits)	(485,33)	(12,3)(7) (60,5)(15) (156,11)(35) (276,19)(61) (660,45)(145) (1572,107)(345) (2748,187)(603) (6540,445)(1435) (15564,1059)(3415)
(5,2) (four orbits)	(31,4)	(20,4)(3) (40,6)(5) (200,26)(23) (340,44)(39)
(5,3) (seven orbits)	(41,4)	(20,4)(4) (50,6)(7) (85,9)(11) (160,16)(20) (295,29) (470,46)(58) (860,84)(106)
(5,4) (eight orbits)	(721,57)	(20,4)(5) (60,6)(9) (300,24)(39) (580,46)(75) (1340,106)(173) (2580,204)(333) (11460,906)(1479) (22060,1744)(2847)
(5,5) (square)	(1,0)	(20,4)(6) (70,6)(11) (155,11)
(5,6) (12 orbits)	(1351,78)	(20,4)(7) (80,6)(13) (160,10)(23) (340,20)(47) (620,36)(85) (1280,74)(175) (2320,134)(317) (4780,276)(653) (8660,500)(1183) (17840,1030)(2437) (32320,1866)(4415) (66580,3844)(9095)
(6,2) (nine orbits)	(55,6)	(12,4)(2) (30,5)(3) (54,7) (114,13)(9) (180,20)(14) (282,31) (558,61)(43) (870,95)(67) (1356,148)
(6,3) (square)	(1,0)	(30,5)(4) (66,7) (222,19)
(6,4) (12 orbits)	(485,33)	(30,5)(5) (78,7) (114,9)(11) (210,15)(19) (510,35)(45) (894,61) (1218,83)(107) (2130,145)(187) (5070,345)(445) (8862,603) (12066,821)(1059) (21090,1435)(1851)
(6,5) (12 orbits)	(1351,78)	(30,5)(6) (90,7)(10) (210,13)(20) (390,23)(36) (810,47)(74) (1470,85)(134) (3030,175)(276) (5490,317)(500) (11310,653)(1030) (20490,1183)(1866) (42210,2437)(3844) (76470,4415)(6964)
(6,6) (eight orbits)	(199,10)	(30,5)(7) (102,7) (366,19)(35) (690,35)(65) (1290,65)(121) (2406,121) (7422,373)(695) (13830,695)(1295)

$$(k,y) = (u_2 + 1, u_1 - 1) \in \mathbb{S}(u_1,u_2). \tag{5.7}$$

showing that the set $\mathbb{S}(u_1,u_2)$ is never empty; on the other hand, the point (5.7) does not satisfy the threshold condition (5.5b). It is, however, true that

$$h_0^{-1}(u_2 + 1, u_1 - 1) < h_0(u_2 + 1, u_1 - 1), \tag{5.8a}$$

$$h_0(u_2 + 1, u_1 - 1) \geqslant (u_2 + 3, u_1 + 3) \tag{5.8b}$$

for $u_1 \geqslant 2$, $u_2 \geqslant 2$, which proves (5.6). Relation (5.8a) is trivial to prove; (5.8b) may be proved directly from the definition (4.12b) of h_0, using the property $v_0 \geqslant 1$, $u_0 > u_1 + 1$ of the least positive solution of $u^2 - Dv^2 = 1$ for $u_1 \geqslant 2$, $u_2 \geqslant 2$ and D nonsquare.

The orbit $H_0(k,y)$ of the point $(k,y) \in \mathbb{S}(u_1,u_2)$ under the action of the group H_0 is, by definition, the set of points

$$H_0(k,y) = \{h_0^n(k,y) \mid n \in \mathbb{Z}\}. \tag{5.9}$$

The results above furnish the complete answer to the problem of obtaining all weight-2 zeros of the $3j$ coefficient in terms of Pell's equation. We state this result as a theorem, using the notations above.

Theorem 5.2: For each pair $(u_1,u_2) \in \mathbb{N}^2$ with $u_1 \geqslant 2$, $u_2 \geqslant 2$, we have

$$\begin{bmatrix} 2 & x_1 & x_2 + u_1 - 2 \\ u_1 + u_2 - 2 & x_2 & x_1 - u_2 + 2 \\ x_1 + x_2 - u_2 & u_1 & u_2 \end{bmatrix} = 0, \tag{5.10}$$

where the integer pair $(x_1,x_2) \in \mathbb{N}^2$ with $x_1 \geqslant u_2$, $x_2 \geqslant 2$ is any of the pairs given by

$$x_1 = (k' + u_2 - 3)/2, \tag{5.11a}$$

$$x_2 = (y' - u_1 + 1)/2, \tag{5.11b}$$

for each (k',y') such that

$$(k',y') \in H_0(k,y), \tag{5.12a}$$

$$(k',y') \geqslant (k^*,y^*), \tag{5.12b}$$

in which the point (k,y) itself runs over all elements in the set $\mathbb{S}(u_1,u_2)$.

Remark: the Regge symmetries and Theorem 5.2 give *all* nontrivial weight-2 zeros of the $3j$ coefficients in terms of positive solutions of the Pell equation. Because of parity, modular, and threshold restrictions, not all solutions of the Pell equation map back to weight-2 zeros. In the final result, given by Theorem 5.2, the zeros (5.10) are classified according to the orbits $H_0(k,y)$, where (k,y) is a point in $\mathbb{S}(u_1,u_2)$, there being an orbit for each such point. By construction, each point (x',y') in the orbit $H_0(k,y)$ has parity such that the pair (x_1,x_2) is integral, but not necessarily positive nor greater than the threshold required to make all entries in the Regge array greater than 2. The condition $(k',y') \geqslant (k^*,y^*)$ assures this property for the corresponding points (x_1,x_2).

It is useful to illustrate the results given here and in Sec. IV by an example from Table I. Consider $(u_1,u_2) = (6,2)$, which has $D = 84$ and $N = -1200$. The least positive solution (u_0,v_0) of $u^2 - 84v^2 = 1$ is $(u_0,v_0) = (55,6)$, which gives

$$g_0 = \begin{pmatrix} 55 & 504 \\ 6 & 55 \end{pmatrix}. \tag{5.13}$$

The set $\mathbb{D}(6,2)$ of fundamental solutions of $x^2 - 84y^2 = -1200$ is

$$\mathbb{D}(6,2) = \left\{ \begin{matrix} (12,4), & (30,5), & (54,7), & (114,13), & (180,20) \\ (282,31), & (558,61), & (870,95), & (1356,148) & \end{matrix} \right\}. \tag{5.14a}$$

The set of all solutions belonging to the positive branch $y > 0$ is

$$\{ g_0^n \mathbb{D}(6,2) \mid n = 0, \pm 1, \ldots \}, \tag{5.14b}$$

or, equivalently, it consists of the set of nine orbits

$$\{ G_0(x,y) \mid (x,y) \in \mathbb{D}(6,2) \}. \tag{5.14c}$$

The subset $\mathbb{A}(6,2) \subset \mathbb{D}(6,2)$ of fundamental solutions whose points satisfy $x + 12y = 0 \bmod 30$ is

$$\mathbb{A}(6,2) = \left\{ \begin{matrix} (12,4), & (30,5), & (114,13), & (180,20) \\ (558,61), & (870,95) & & \end{matrix} \right\} \tag{5.15}$$

with the corresponding set $\mathbb{B}(6,2)$ of values (k,y) given by

$$\mathbb{B}(6,2) = \left\{ \begin{matrix} (2,4), & (3,5), & (9,13), & (14,20) \\ (43,61), & (67,95) & & \end{matrix} \right\}. \tag{5.16}$$

Finally, the subset $\mathbb{S}(6,2)$ of points in $\mathbb{B}(6,2)$ having the proper parity is

$$\mathbb{S}(6,2) = \{(3,5), (9,13), (43,61), (67,95)\}. \tag{5.17}$$

The group H_0 is given by

$$H_0 = \{ h_0^n \mid n = 0, \pm 1, \pm 2, \ldots \}, \tag{5.18a}$$

where

$$h_0 = \begin{pmatrix} 127 & -12 \\ 180 & -17 \end{pmatrix}. \tag{5.18b}$$

The orbits of the group H_0 on the set $\mathbb{S}(6,2)$ are

$$H_0(3,5), H_0(9,13), H_0(43,61), H_0(67,95). \tag{5.19}$$

We see that there are four disjoint denumerably infinite families of weight-2 zeros of the $3j$ coefficients corresponding to $(u_1,u_2) = (6,2)$. These zeros are given by the Regge array

$$\begin{bmatrix} 2 & (k'-1)/2 & (y'+3)/2 \\ 6 & (y'-5)/2 & (k'-1)/2 \\ (k'+y'-10)/2 & 6 & 2 \end{bmatrix} = 0, \tag{5.20}$$

where (k',y') is a positive point in any of the four orbits (5.19) satisfying $(k',y') \geqslant (5,9) = (k^*,y^*)$. This includes, in fact, all points in the orbits (5.19) with the exception of the four points:

$$(1,5) = h_0^{-1}(67,95) \in H_0(67,95),$$
$$(1,7) = h_0^{-1}(43,61) \in H_0(43,61),$$
$$(3,31) = h_0^{-1}(9,13) \in H_0(9,13),$$
$$(3,5) = h_0^{0}(3,5) \in H_0(3,5).$$

The result for weight-2 zeros of the $3j$ coefficients as given by Theorem 5.2 is, we believe, a comprehensive and elegant statement of the origin of these zeros in terms of a classical Diophantine equation, the Pell equation.

VI. RELATION TO BINARY QUADRATIC FORMS

We have chosen to solve the Pell equation (3.1) in determining the weight-2 zeros of the $3j$ coefficients. This procedure required rejecting from the set of fundamental solutions those that failed to satisfy the divisibility condition (4.8). This step can be avoided by using a different formulation of the problem. This alternative, but closely related, method is of interest because it relates the properties of the weight-2 $3j$ coefficients directly to those of binary quadratic forms, which is a well-studied subject in number theory.[26–28]

A (real) binary quadratic form $q_{a,b,c}$ is a homogeneous polynomial in $(x,y) \in \mathbb{R}^2$ with coefficients $(a,b,c) \in \mathbb{R}^3$,

$$q_{a,b,c}(x,y) = ax^2 + bxy + cy^2. \tag{6.1}$$

The *discriminant* d of $q_{a,b,c}$ is

$$d = b^2 - 4ac. \tag{6.2}$$

The form is said to be *definite* if $d < 0$; *indefinite* if $d > 0$.

To transform $Q_{u_1,u_2}(x_1,x_2)$ [see Eq. (1.3)] to binary quadratic form, we eliminate only the linear terms. Thus carrying out the transformation

$$(u_1,u_2,x_1,x_2) = U \cdot (u_1,u_2,x,y), \tag{6.3a}$$

$$U = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 & -\frac{3}{2} \\ -\frac{1}{2} & 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \tag{6.3b}$$

we obtain the new polynomial F,

$$F(u_1,u_2,x,y) = Q_{u_1,u_2}(x_1,x_2) = q_{a,b,c}(x,y) - m. \quad (6.4)$$

The coefficients a,b,c are the following functions of u_1,u_2:

$$a = u_1(u_1-1)/2, \quad c = u_2(u_2-1)/2,$$
$$b = -u_1u_2, \quad m = -(u_1-1)(u_2-1)(u_1+u_2)/2. \quad (6.5)$$

The quadratic polynomial $P_{v_1,v_2}(y_1,y_2)$ may be similarly transformed:

$$(v_1,v_2,y_1,y_2) = V\cdot(v_1,v_2,x,y), \quad (6.6a)$$

$$V = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} & 0 & 1 \\ 0 & \frac{1}{2} & 0 & \frac{1}{2} & 1 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad (6.6b)$$

$$G(v_1,v_2,x,y) = P_{v_1,v_2}(y_1,y_2) = q_{a,b,c}(x,y) - m, \quad (6.7)$$

with coefficients

$$a = (v_2+1)(v_2+2)/2, \quad c = (v_1+1)(v_1+2)/2,$$
$$b = (v_1+1)(v_2+1), \quad (6.8)$$
$$m = (v_1+2)(v_2+2)(v_1+v_2+2)/2.$$

The discriminants of these two forms $q_{a,b,c}$ with coefficients (6.5) and (6.8), respectively, are

$$d_1(u_1,u_2) = u_1u_2(u_1+u_2-1), \quad (6.9a)$$

$$d_2(v_1,v_2) = -(v_1+1)(v_2+1)(v_1+v_2+3). \quad (6.9b)$$

Consequently, for $u_1 \geqslant 1$, $u_2 \geqslant 2$ and $v_1 \geqslant 0$, $v_2 \geqslant 0$, the corresponding forms $q_{a,b,c}$ are indefinite and definite, respectively.

In studying the relations between the families of quadratic polynomials described above, we take the various parameters and coordinates to be defined individually on the real line; an n-tuple composed of these is taken to lie in $\mathbf{R}^n$; for example,

$$(u_1,u_2,x,y) \in \mathbf{R}^4. \quad (6.10)$$

With this extension, the relation

$$G(-u_2-1,-u_1-1,-x,y) = F(u_1,u_2,x,y) \quad (6.11)$$

is valid for the full domain (6.10). Consequently, there is only one family of binary quadratic forms occurring here; namely, the form (6.4) with coefficients given by Eqs. (6.5). The discriminants then also agree, $d_2(-u_2-1,-u_1-1) = d_1(u_1,u_2)$.

Relation (1.11) can also be expressed in terms of the variables (6.10). In terms of the transformation W defined by $(v_1,v_2,y_1,y_2) = W\cdot(u_1,u_2,x_1,x_2)$ [see Eqs. (1.9)], U defined by Eqs. (6.3), and V by Eqs. (6.6), the relation between G and F is

$$G(T\cdot(u_1,u_2,x,y)) = F(u_1,u_2,x,y), \quad (6.12a)$$

where

$$T = V^{-1}WU = \begin{pmatrix} 1 & 1 & 0 & 0 & -2 \\ -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & -1 \\ 1 & -1 & 0 & 0 & 0 \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}. \quad (6.12b)$$

Combining relations (6.11) and (6.12) we obtain the following theorem.

Theorem 6.1: The function F is invariant under the transformation S defined by

$$S = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & 0 \\ -1 & -1 & 0 & 0 & 1 \\ -1 & 1 & 0 & 0 & 0 \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}; \quad (6.13a)$$

that is,

$$F(u_1,u_2,x,y) = F(S\cdot(u_1,u_2,x,y)). \quad (6.13b)$$

This symmetry of F is in addition to the eight Regge array symmetries of the group K defined by Eq. (1.15). The latter symmetry is expressed by $F(u_1,u_2,x,y) = F(m\cdot(u_1,u_2,x,y))$, each $m \in M = U^{-1}KU$. In particular, the interchange symmetry $u_1 \leftrightarrow u_2$, $x \leftrightarrow y$ of F is the transformation $U^{-1}rU$.

The group M' generated by the group M and the transformation S is a finite group of symmetries of the function F. This group will be described in detail in another paper dealing with the general symmetry group of the "polynomial part" of a $3j$ coefficient.

The group M' is the same for all $(u_1,u_2,x,y) \in \mathbf{R}^4$; that is, the group elements do not depend on the point in $\mathbf{R}^4$. The function F has, in addition, *a continuous group of symmetries at each point* $(u_1,u_2) \in \mathbf{R}^2$. The nature of this group depends on the point (u_1,u_2). Since this group structure belongs to an arbitrary binary quadratic form $q_{a,b,c}(x,y)$ defined by Eq. (6.1), we give its general formulation.

We define the graph $\mathbf{A}_d$ of the function $u^2 - dv^2 = 1$ by

$$\mathbf{A}_d = \{(u,v) \mid u^2 - dv^2 = 1\}, \quad (6.14)$$

where d is the discriminant of $q_{a,b,c}$. To each point $(u,v) \in \mathbf{A}_d$, we let correspond the 2×2 unimodular matrix

$$h(u,v) = \begin{pmatrix} u-bv & -2cv \\ 2av & u+bv \end{pmatrix}, \quad (6.15)$$

where a,b,c are the coefficients in $q_{a,b,c}$, which we regard as specified. Then the set H defined by

$$H = \{h(u,v) \mid (u,v) \in \mathbf{A}_d\} \quad (6.16)$$

is a group under matrix multiplication, which may also be expressed as $h(u,v)h(u',v') = h(uu' + vv'd, uv' + vu')$; the identity is $h(1,0)$, and $h(u,v)^{-1} = h(u,-v)$. [Here the coefficients have been suppressed in writing H and $h(u,v)$.]

The principal result for the group H, which may be proved by direct substitution, is the following.

Theorem 6.2: The group H is an invariance group of the binary quadratic form $q_{a,b,c}$; that is,

$$q_{a,b,c}(x',y') = q_{a,b,c}(x,y), \quad (6.17a)$$

for

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = h \begin{pmatrix} x \\ y \end{pmatrix}, \quad \text{each } h \in H. \quad (6.17b)$$

It is not difficult to prove that H is isomorphic to the Lorentz group $SO(1,1)$ for $d>0$, to the rotation group $SO(2)$ for $d<0$, and to a group $\Delta(2)$ of 2×2 triangular matrices for $d=0$.

The invariance group H is important for the study of the Diophantine equation

$$q_{a,b,c}(x,y) = m, \tag{6.18}$$

where now $(a,b,c,x,y) \in \mathbb{Z}^5$ and $m \in \mathbb{Z}$ is in the range of $q_{a,b,c}$. The group H is significant because of its integer subgroups: integer points $(u,v) \in \mathbb{A}_d$ correspond to elements $h(u,v) \in H$ with integer entries, and such elements of H map integer solutions of (6.18) to integer solutions. Not all integer elements of H, however, lead to distinct solutions. This is because all integer solutions of $u^2 - dv^2 = 1$ belong to a single orbit of the group $\{G_0, -G_0\}$, where G_0 is defined by Eq. (3.5) with $D = d = b^2 - 4ac$. The implication of this result is that only the subgroup $H_0 = \{h_0^n | n \in \mathbb{Z}\} \subset H$, where

$$h_0 = \begin{pmatrix} u_0 - bv_0 & -2cv_0 \\ 2av_0 & v_0 + bv_0 \end{pmatrix}, \tag{6.19}$$

is relevant in the classification of the set of solutions of Eq. (6.18) by the orbits of $\{H_0, -H_0\}$.

Let $(x,y) \in \mathbb{Z}^2$ be a solution of Eq. (6.18), if such exists. We can define a fundamental solution with respect to H_0 to be the least positive solution in the orbit $\pm H_0(x,y)$. (Any set of orbit representatives could serve as a set of fundamental solutions.) In this way, the problem of finding all integer solutions of Eq. (6.18) is reduced to that of finding the fundamental ones, which are always finite in number (including zero). For $d > 0$ and nonsquare (hyperbolic case), the matrix h_0 generates an infinite-order discrete group $H_0 \subset SO(1,1)$, and the infinitely many solutions of Eq. (6.18) are classified by a finite number of orbits $\pm H_0(x,y)$, one for each fundamental solution (x,y). For $d > 0$ and square (hyperbolic case) or for $d < 0$ (elliptical case), we have $(u_0,v_0) = (1,0)$ so that $h_0 = H_0 = I$, the identity matrix. The invariance groups $\{I, -I\} \subset SO(1,1)$ and $\{I, -I\} \subset SO(2)$ now yield only the points (x,y) and $(-x,-y)$ in the same orbit.

In the application of the preceding results on binary quadratic forms to the special forms with coefficients (6.5) and (6.8), an extra richness of structure appears. This is brought out nicely by considering the surface $\mathbb{F}$ in $\mathbb{R}^4$ defined by

$$\mathbb{F} = \{(u_1,u_2,x,y) \in \mathbb{R}^4 | F(u_1,u_2,x,y) = 0\}. \tag{6.20}$$

The set of *lattice points* $\mathbb{L}$ of this surface is the set of points of $\mathbb{F}$ with integer coordinates,

$$\mathbb{L} = \{(u_1,u_2,x,y) \in \mathbb{Z}^4 | F(u_1,u_2,x,y) = 0\}. \tag{6.21}$$

In particular, the set $\mathbb{L}$ contains all points that correspond to weight-2 zeros of the $3j$ coefficients, both in the hyperbolic and elliptical classifications [see Eqs. (6.3), (6.4), (6.6), (6.7), and (6.11)]. Unlike the general case (6.18), the set $\mathbb{L}$ is never empty, since it always contains the points

$$(u_1,u_2,u_2+1,u_1-1), \text{ all } (u_1,u_2) \in \mathbb{Z}^2,$$

and

$$(u_1,u_2,u_2+1+(4u_2/(u_1-1)),u_2+1), \text{ all } (u_1,u_2) \in \mathbb{Z}^2$$

such that $u_1 - 1$ divides $4u_2$.

Each (u_1,u_2) plane in $\mathbb{F}$ has a symmetry group that is either isomorphic to $SO(1,1)$ $(d > 0)$, to $SO(2)$ $(d < 0)$, or to $\Delta(2)$ $(d = 0)$. If we restrict the surface $\mathbb{F}$ to its subset of lattice points $\mathbb{L}$, the relevant group for the (u_1,u_2) plane, with $(u_1,u_2) \in \mathbb{Z}^2$, is restricted to the discrete subgroup $\{H_0, -H_0\}$, so that all points in $\mathbb{L}$ can be classified by orbits relative to this subgroup. (This is, to be sure, a rather trivial classification in some cases.)

In addition to the group structure of points in a (u_1,u_2) plane described above, there is also the symmetry of the surface $\mathbb{F}$ corresponding to the transformations belonging to the finite group M' (see Theorem 6.1 *et seq.*) These transformations map points from one (u_1,u_2) plane to another. The following example illustrates this property.

Take $(u_1,u_2) = (6,2)$. This is our earlier example [see Eqs. (5.13)–(5.18)] rephrased in terms of binary quadratic forms. We have

$$F(6,2,x,y) = 15x^2 - 12xy + y^2 + 20 = 0. \tag{6.22}$$

The (6,2) plane in $\mathbb{L}$ contains an infinite number of lattice points given by the orbits $\pm H_0(x_1,y_1)$, where $(x_1,y_1) \in \mathbb{B}(6,2)$. These orbits, of course, constitute all integer solutions of Eq. (6.22).

Under the transformation S given by (6.13a), an integer solution (x,y) of (6.22) is mapped to an integer solution of

$$F(u_1',u_2',x',y') = 0, \tag{6.23a}$$

where

$$(u_1',u_2') = (4 - \tfrac{1}{2}(x+y), -7), \tag{6.23b}$$

$$(x',y') = (-4, 2 + \tfrac{1}{2}(x-y)). \tag{6.23c}$$

The point (u_1',u_2',x',y') belongs to $\mathbb{L}$. The original (6,2) plane is, however, hyperbolic, while for $|x+y| \geq 10$, the (u_1',u_2') plane is elliptical. The integer solutions (infinite in number) of

$$q_{15,-12,1}(x,y) = -20 \tag{6.24a}$$

are distributed by the map S into integer solutions, one each, of the infinite number of Diophantine equations.

$$q_{a',b',c'}(-4, 2 + \tfrac{1}{2}(x-y)) = m', \tag{6.24b}$$

where a',b',c', and m' are expressed in terms of (u_1',u_2') by Eqs. (6.5).

The properties of the function $F(u_1,u_2,x,y)$ discussed in this section are intended only to indicate the deep structure associated with the polynomial part of a $3j$ coefficient. We have not implemented methods discussed in Refs. 26–28 of solving the Diophantine equation $F(u_1,u_2,x,y) = 0$, since from a calculational viewpoint this would repeat much of Secs. III–V, which have been based directly on Pell's equation.

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Construction of space-time by gauge translations

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The following procedure is described: Starting with a connection in a principal fiber bundle $P(M,G)$, where G is either the Poincaré group or one of the de Sitter groups, a connection in the bundle of linear frames of a submanifold N of M is constructed by using the translational components of the original connection for frame identification. The dimension of N is gauge dependent, and the flat four-dimensional Minkowski space-time may appear of dimension less than 4 when certain gauges are used. It is shown that in the case of a de Sitter group, the minimum dimension to which the flat four-dimensional space-time can be reduced is 1, while the number is 0 for the Poincaré group. The gauge transformation that achieves the maximum dimension reduction in the de Sitter case is constant and leads to infinite strings as a result. Variable continuous gauge transformations that can reduce the dimension over a finite region of the base manifold are also considered.

I. INTRODUCTION

Ever since Kibble[1] proposed a theory with translations included in the gauge group of general relativity, the subject has been extremely popular. The emphasis has been, however, on the introduction of torsion into general relativity (Riemann–Cartan geometry) and the construction of Lagrangians. Some examples of the literature are given in Ref. 2.

In this paper it is the geometry of the construction that is primarily studied, expanding a short note listed in Ref. 3. The main geometric role played by the translations in the gauge group is that it can provide the necessary "soldering,"[4] i.e., it changes a principal fiber bundle with no special relationship between the points on the fibers and the base manifold into the bundle of linear frames of the base manifold. The soldering is based on an identification of the translational component of the original connection form with the canonical form of the bundle of linear frames. The identification is made on a partially fixed cross section subject only to Lorentz gauge transformations. Since the Poincaré group and de Sitter groups are indistinguishable as far as the adjoint action of the Lorentz subgroup is concerned, the soldering can be done in the same way for all three cases. However, the procedure depends on the selection of the reference cross section, and that is where the difference between the Poincaré and the de Sitter groups shows up. When the rank of the translational component of the connection form is less than 4, full soldering is not possible, but in some cases it can still be carried out on a submanifold of the base manifold. In particular, a connection may yield the flat four-dimensional space-time in one gauge, and a space of a lower dimension in another gauge. One can ask about the minimum dimension to which the flat four-dimensional space-time can be reduced by a transformation. In the de Sitter case, which is, in general, geometrically more interesting than the Poincaré case, the minimum dimension is 1. This could be somehow connected with the fact that the most elementary constituents of matter seem to have the appearance of one-dimensional strings.

Section II introduces the construction of a bundle of linear frames from the principal fiber bundle with Poincaré or de Sitter structure using the formalism of the modern differential geometry.[5] Section III discusses a physical interpretation of the construction. Section IV describes explicitly the construction of Sec. II in terms of coordinates, while Sec. V is concerned with the construction of a flat Minkowski space and its gauge dependence. Section VI gives an example of a partial dimension reduction in spherical coordinates.

II. SOLDERING BY GAUGE TRANSLATIONS

Chapter III of Ref. 5 describes the reduction of the bundle of affine frames to the bundle of linear frames and the affine connection. Since it is closely related to the construction described later, it will be briefly reviewed. A linear frame of an n-dimensional manifold M is a basis $(X_1,...,X_n)$ of the tangent vector space $T_x(M)$ at $x \in M$. An affine frame is a linear frame together with a point in $T_x(M)$ regarded as an affine space. There is a natural map from the bundle of linear frames $L(M)$ into the bundle of affine frames $A(M)$ defined by

$$\gamma(X_1,...,X_n) = (0_x;X_1,...,X_n)\,, \tag{2.1}$$

where 0_x is the origin of $T_x(M)$. If $\tilde{\omega}$ is a connection form on $A(M)$ then its image on $L(M)$ splits naturally into $\mathrm{Gl}(n,\mathbb{R})$ components,

$$\gamma^*\tilde{\omega} = \omega + \phi\,. \tag{2.2}$$

Every linear frame $(X_1,...,X_n)$ at $x \in M$ can be considered as a linear map u of $\mathbb{R}^n$ onto $T_x(M)$ by

$$u(a^1,...,a^n) = \sum_{i=1}^{n} a^i X_i\,. \tag{2.3}$$

The canonical form θ on $L(M)$ is the $\mathbb{R}^n$-valued form defined by

$$\theta(X) = u^{-1}(\pi(X))\,, \tag{2.4}$$

where X is a tangent vector in the bundle manifold of $L(M)$, and π is the canonical projection in $L(M)$ from the bundle manifold to the base manifold. It is easy to see that

$$(R_a^*\theta)(X) = a^{-1}(\theta(X))\,, \tag{2.5}$$

where R_a is the right action of $a \in \mathrm{Gl}(n,\mathbb{R})$ on $L(M)$. Since the form defined by (2.2) has the same transformation law

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(2.5) as θ, it is possible to define an affine connection in $A(M)$ as a connection for which $\phi = \theta$. The curvature form $\tilde{\Omega}$ of an affine connection in $A(M)$ decomposes under the injection γ defined by (2.1) according to

$$\gamma^* \tilde{\Omega} = \Omega + \Theta , \tag{2.6}$$

where Ω and Θ are, respectively, the curvature and torsion forms on $L(M)$.

If an affine connection in $A(M)$ is reducible to a Poincaré type subgroup of the affine group, then the linear connection in $L(M)$ is reducible to the corresponding Lorentz type subgroup of $\mathrm{Gl}(n, \mathbb{R})$.

The aim of this section is to use the above for defining a construction of a bundle of linear frames from a principal fiber bundle $P(M,G)$, where M is a four-dimensional manifold, and G is the Poincaré group. Only local aspects of the construction will be considered in this paper. Thus the bundle manifold P can be considered as $M \times G$, and a subbundle $Q(M,H)$ of P can be identified. Here $Q = M \times H$ and H is the Lorentz subgroup of G. If γ is the natural injection of Q into P and $\tilde{\omega}$ is a connection form on P,

$$\gamma^* \tilde{\omega} = \omega + \theta , \tag{2.7}$$

where ω and θ are forms on Q with values in the Lorentz algebra and $\mathbb{R}^n$, respectively. Under the right action of $a \in H$, θ behaves exactly as in (2.5). It can thus be identified with a canonical form of a bundle of linear frames, which is already reduced to a Lorentz structure. By the identification it is meant that (2.4) is used to determine u^{-1}, which in its turn defines the frames by (2.3). To ensure the existence of u we must have a condition

$$\theta(X) = 0 \Rightarrow \pi(X) = 0 . \tag{2.8}$$

Let us now assume that

$$\theta(X) = 0 \quad \text{if } \pi(X) \in U_x , \tag{2.9}$$

where U_x is a subspace of $T_x(M)$. Selecting another subspace V_x of $T_x(M)$ such that

$$T_x(M) = U_x \oplus V_x \quad \text{and} \quad \theta(X) \neq 0 \quad \text{if } \pi(X) \neq 0 \quad \text{and} \quad \pi(X) \in V_x ,$$

an invertible map $v^{-1}: V_x \to \mathbb{R}^p$ can be defined by

$$\rho(\theta(X)) = v^{-1}(\pi(X)), \quad \pi(X) \in V_x , \tag{2.10}$$

where ρ is a canonical projection $\mathbb{R}^4 \to \mathbb{R}^p, p = \mathrm{Dim}\, V_x$. If V_x defines an involutive distribution on M then there exists (locally) a submanifold N of M such that $T_x(N) = V_x$. In that case map v can be used to define linear frames on N. A connection in $L(N)$ is defined by ω with values restricted to the subgroup of the Lorentz group determined by projection ρ.

Several comments about the above described construction are in order.

(i) Depending on the original connection in $P(M,G)$ it may or may not be possible to construct submanifold N. When the construction is possible, it is in general not unique. The dimension of N, however, is unique since it is determined by the rank of θ.

(ii) The construction does not work only for the Poincaré group in the role of G. If G is ten-dimensional and its Lie algebra can be written as

$$\mathsf{G} = \mathsf{H} \oplus \mathsf{T} , \tag{2.11}$$

where H is the Lie algebra of the Lorentz group and T is an h-dimensional subspace of G that transforms under the adjoint map ad H in the same way as the translations in the Poincaré group, then G can be used for the construction. Indeed, injection γ will still exist, $\gamma^* \tilde{\omega}$ will still decompose as in (2.7), and it will still have the correct behavior under the right action of H. Since the construction is on the subbundle $Q(M,H)$, the Lie aglebraic properties of T are not important, except for its transformation under ad H. In this way G can be also a de Sitter group of type either (4,1) or (3,2).

(iii) The construction may be possible also when M has dimension higher than 4. Since θ can have rank at most 4, some dimension reduction must occur, and the success of the construction will depend on the existence of the involutive distribution V_x.

(iv) Most importantly, the construction depends on the particular way in which P is represented as $M \times G$. Such a representation involves a selection of a reference cross section corresponding to the identity element of G. In physical applications this is called gauge, and a change from one reference cross section to another is called a gauge transformation. Gauge invariance of the construction is retained only as far as a Lorentz gauge transformation is concerned (or the appropriate subgroup of the Lorentz group in case of a lower dimension), but a gauge transformation involving translations can change the result, including the final dimension of the constructed submanifold. Gauge dependent results are usually not studied in differential geometry. After all, a gauge transformation is just a special kind of a coordinate transformation, and the true modern differential geometry is concerned only with the properties that can be described in a coordinate-free fashion. Alas, in physical applications the selection of a gauge and gauge transformations often play an important role and, as discussed in the next section, the role could be crucial in case of translations.

III. PHYSICAL INTERPRETATION

Before the construction described in Sec. II is demonstrated on particular examples, let us discuss the physical motivation and interpretation of the results. For a physical understanding of concepts like connection and reference cross section, it is better to introduce the connection via the horizontal lift, rather than the connection form.

If $P(M,G)$ is a principal fiber bundle with a connection form ω, the horizontal lift $X^{(h)}$ of $X \in T_x(M)$ is the unique tangent vector at $p \in P$, $x = \pi(p)$, satisfying

$$\pi(X^{(h)}) = X \quad \text{and} \quad \omega(X^{(h)}) = 0 . \tag{3.1}$$

Physically, transport in the horizontal direction implies no measurable change of the geometrical properties described by G. For example, if $P(M,G)$ were a bundle of linear frames of a three-dimensional manifold and G the group of rotations, a frame transported in the horizontal direction would be perceived as parallel to the original frame, i.e., without any observable rotation.

Thus $\theta(X) = 0$ of Sec. II can be interpreted as "no observable translation" in the direction of $\pi(X)$. Dimension of

M is then just the number of parameters needed to describe physical fields, while the dimension of the submanifold N is the observable physical dimension. Our macroscopical experience with space-time tells us that the observable dimension is 4. Since the dimension depends on the selected reference cross section (gauge), it must be assumed that the gauge is to some extent fixed. It is not too surprising, since even the Lorentz gauge, though theoretically free to choose, would be difficult to set up practically if its Lorentz frames involved high velocities. Hence it is possible that our macroscopical methods of measuring space-time intervals restrict us to a fixed gauge as far as translations are concerned. Such restrictions may not apply in the microworld of elementary particles, where the same space-time may appear to have a different dimension due to the fact that it is viewed from a different gauge.

IV. EXPRESSION IN LOCAL COORDINATES

To investigate particular cases one has to formulate everything explicitly, using local coordinate systems.

Let M be a four-dimensional manifold with a local coordinate system $(x^\mu, \mu = 1,...,4)$. Consider a principal fiber bundle $P(M,G)$, where G is either the Poincaré group or one of the de Sitter groups. In a particular gauge, a connection in P can be defined by the horizontal lift of $\partial/\partial x^\mu \in T_x(M)$,

$$X^{(h)}_\mu = \frac{\partial}{\partial x^\mu} - \frac{1}{2} A^{ij}_\mu(x) W_{ji} - A^i_\mu(x) T_i \,. \tag{4.1}$$

Here W_{ji} and T_i are the right invariant vector fields in G, with W_{ji} spanning the Lorentz algebra. Functions $A^{ij}_\mu(x)$ are the Lorentz components of the connection, while $A^i_\mu(x)$ correspond to the form θ of (2.7) by

$$\theta^i(X^{(h)}_\mu) = A^i_\mu(x) \,. \tag{4.2}$$

The coordinates in the Poincaré group can be chosen as the elements of 5×5 matrices

$$\begin{bmatrix} X^i_j & 0 \\ Y_j & 1 \end{bmatrix}, \tag{4.3}$$

where

$$\begin{aligned} &X^i_j g_{il} X^l_k = g_{jk} \,, \\ &g_{jk} = \mathrm{diag}(1,1,1,-1) \,. \end{aligned} \tag{4.4}$$

The right-invariant vector fields are then

$$W_{ij} = g_{ik} W^k_j - g_{jk} W^k_i, \quad W^k_j = X^k_m \frac{\partial}{\partial X^j_m}, \tag{4.5}$$

and

$$T_i = g_{ij} X^j_k \frac{\partial}{\partial Y_k} \,. \tag{4.6}$$

The coordinates in a de Sitter group can be chosen as the elements of 5×5 matrices $[X^p_q]$ satisfying

$$\begin{aligned} &X^p_r g_{pq} X^q_s = g_{rs} \,, \\ &g_{rs} = \mathrm{diag}(1,1,1,-1,\pm 1) \,. \end{aligned} \tag{4.7}$$

The right-invariant vector fields are then

$$W_{pq} = g_{pr} W^r_q - q_{qr} W^r_p, \quad W^r_p = X^r_s \frac{\partial}{\partial X^p_s}, \tag{4.8}$$

where the restriction of indices to the range 1, 2, 3, 4 defines W_{ij}, while

$$T_i = W_{5i} \,. \tag{4.9}$$

A gauge transformation is characterized by the right action of group G on the reference cross section with the group element being a function of position in M. This causes a change of the coordinate system in $P = M \times G$ with the new coordinates in G measuring the position on the fibers from the new cross section. If the variable group elements are characterized by $a^i_j(x)$ and $a_j(x)$ in case of the Poincaré case and by $a^p_q(x)$ in the de Sitter cases, the respective transformations are

$$\begin{aligned} &\bar{x}^\mu = x^\mu, \quad \bar{X}^i_j = b^i_k(x) X^k_j \,, \\ &\bar{Y}_j = Y_j - a_i(x) b^i_k(x) X^k_j \,, \end{aligned} \tag{4.10}$$

and

$$\bar{X}^p_q = b^p_r(x) X^r_q \,. \tag{4.11}$$

Here matrices $[b^i_j]$ and $[b^p_q]$ are inverses of $[a^i_j]$ and $[a^p_q]$.

Applying the transformations (4.10) and (4.11) to the horizontal lift (4.1) yields the gauge transformation of the connection components.

For the Poincaré case

$$\begin{aligned} \bar{A}^{ij}_\mu &= b^i_k A^{kl}_\mu b^j_l + (\partial_\mu b^j_k) b^i_l g^{kl} \,, \\ \bar{A}^i_\mu &= b^i_k A^k_\mu + b^i_k A^{kl}_\mu b^j_l a_j + g^{jl}(\partial_\mu a_l) \\ &\quad + g^{jl} b^k_l (\partial_\mu b^j_k) a_j \,. \end{aligned} \tag{4.12}$$

For the de Sitter case

$$\bar{A}^{pq}_\mu = b^p_r A^{rs}_\mu b^q_s + (\partial_\mu b^q_r) b^p_s g^{rs} \,, \tag{4.13}$$

where

$$A^{i5}_\mu \equiv A^i_\mu \text{ of (4.1)} \,.$$

Restricting the gauge transformation to the Lorentz subgroup means $a_j(x) = 0$ for the Poincaré group, and $a^i_5(x) = a^5_j(x) = 0$, $a^5_5(x) = 1$ for the de Sitter groups. Of course, the transformation of A^i_μ is then identical in all cases and given by

$$\bar{A}^i_\mu(x) = b^i_k(x) A^k_\mu(x) \,, \tag{4.14}$$

which is just an explicit expression for the transformation (2.5) of the canonical form.

Curvature of the connection in P can be calculated by taking the commutator

$$[X^{(h)}_\mu, X^{(h)}_\nu] = \tfrac{1}{2} R^{ij}_{\mu\nu} W_{ji} + S^i_{\mu\nu} T_i \,. \tag{4.15}$$

The two terms on the right-hand side of (4.15) correspond to the decomposition (2.6).

V. FLAT SPACE CONSTRUCTION AND ITS GAUGE DEPENDENCE

Let us now assume that in a particular gauge the connection describes a flat Minkowski space. Explicitly it means that the connection is described by a horizontal lift of the form

$$X^{(h)}_\mu = \frac{\partial}{\partial x^\mu} - A^i_\mu(x) T_i \,, \tag{5.1}$$

where the matrix $[a^i_\mu]$ is invertible for all x, and

$$\partial_\mu A^i_\nu - \partial_\nu A^i_\mu = 0 . \tag{5.2}$$

Here $A^i_\mu(x)$ are proportional to the partial derivatives of Minkowski coordinates x^i, $i = 1,...,4$, with respect to general coordinates x^μ, $\mu = 1,...,4$. If the coordinates are considered as measured in units of length, we can write

$$A^i_\mu(x) = \frac{1}{l}\frac{\partial x^i}{\partial x^\mu}, \tag{5.3}$$

where l is a constant length.

Calculating the curvature of the connection defined by (5.1), according to (4.15) one obtains

$$R^{ij}_{\mu\nu} = S^i_{\mu\nu} = 0 \tag{5.4}$$

for the Poincaré group and

$$R^{ij}_{\mu\nu} = \pm (A^i_\nu A^j_\mu - A^i_\mu A^j_\nu), \quad S^i_{\mu\nu} = 0 \tag{5.5}$$

for the de Sitter groups. The curvature of the connection in $L(M)$ generated according to the construction described in Sec. II is, of course, 0 in both cases.

Under a gauge transformation the components of the curvature in (4.15) transform according to the action of ad $a^{-1}(x)$, $a(x) \in G$. In the Poincaré case, $R^{ij}_{\mu\nu}$ and $S^i_{\mu\nu}$ remain 0 in all gauges. For de Sitter groups

$$\overline{S}^i_{\mu\nu} = \pm b^i_k (A^k_\nu A^l_\mu - A^k_\mu A^l_\nu) b^5_l , \tag{5.6}$$

and requirement $\overline{S}^i_{\mu\nu} = 0$ leads to $b^5_l = 0$, $b^l_5 = 0$, and $b^5_5 = 1$. Thus only a Lorentz gauge transformation is permitted if $S^i_{\mu\nu}$ is to remain 0. At the same time, the induced connection in $L(M)$ is not changed by Lorentz gauge transformations. Thus in the de Sitter case, the flat connection in $L(M)$ with $S^i_{\mu\nu} = 0$ is unique. The geometric meaning of $S^i_{\mu\nu}$ in $L(M)$ is that of torsion. Hence we can state the following.

If a flat connection is generated from a connection in $P(M,G)$ with G being a de Sitter group, the gauge is determined up to a Lorentz gauge transformation by the requirement of zero torsion.

This is quite pleasing from the physical point of view, since it hints on a possible relationship between space-time measurements and the choice of the gauge. Macroscopical measurements of space and time are based on the use of geodesics (light rays) and a connection constructed from geodesics (using the Schild's ladder) comes automatically with zero torsion.[6]

Let us now investigate how the dimension of submanifold N constructed from the connection described by (5.1) depends on the choice of the gauge. In particular, we should be interested in the minimum dimension to which the flat four-dimensional space-time can be reduced, and in the gauge that can achieve the maximum reduction.

In the Poincaré case the answer is rather trivial. Using Minkowski coordinates ($A^i_\mu = (1/l)\delta^i_\mu$), $\overline{A}^i_\mu = 0$ in (4.12) leads to

$$b^i_k = \delta^i_k, \quad a_l = -(1/l) g_{lk} x^k . \tag{5.7}$$

Thus the rank of θ is 0, and so is the minimum dimension. This is not surprising, since the original connection in $P(M,G)$ is flat.

In the de Sitter case it is easy to see that the minimum dimension must be greater than 0. Namely, assume that it is 0. Then the horizontal lift (4.1) has only the Lorentz component in the appropriate gauge. But then the curvature has also only the Lorentz component, and that is impossible since $S^i_{\mu\nu}$ can be 0 only in the original gauge. Thus the minimum dimension must be at least 1. The direct way to show that it is in fact equal to 1 is to solve the equations $\overline{A}^{i5}_\mu = 0$, $i = 1,...,4$, for as many values of index μ as possible. Separating index 5 from the remaining values Eq. (4.13) reads

$$\overline{A}^i_\mu = b^j_k A^k_\mu b^5_5 - b^i_5 A^k_\mu b^5_k + (\partial_\mu b^5_5) b^i_5 g^{55} + (\partial_\mu b^5_j) b^i_k g^{jk} = 0 . \tag{5.8}$$

Working in Minkowski coordinates we have for, say $\mu = 1$,

$$(1/l) b^i_l b^5_5 - (1/l) b^i_5 b^5_1 + b^i_5 (\partial_1 b^5_5) g^{55} + b^i_k (\partial_1 b^5_j) g^{jk} = 0 . \tag{5.9}$$

After multiplication by matric $[a^p_q]$ one obtains

$$(1/l)\delta^p_1 - (1/l)\delta^p_5 b^5_1 + \delta^p_5 (\partial_1 b^5_5) g^{55} + g^{pj} (\partial_1 b^5_j) = 0 ,$$

for $p = 1,...5$, which can be written as

$$\begin{aligned} &(1/l) b^5_5 + g^{11} (\partial_1 b^5_1) = 0 , \\ &-(1/l) b^5_1 + g^{55} (\partial_1 b^5_5) = 0 , \\ &\partial_1 b^5_2 = \partial_1 b^5_3 = \partial_1 b^5_4 = 0 . \end{aligned} \tag{5.10}$$

Similar sets of equations must be valid for every dimension μ for which $\overline{A}^i_\mu = 0$. If only one more dimension is added, say $\mu = 2$, the resulting set of equations leads to $b^5_1 = b^5_2 = b^5_5 = 0$. The process can be extended by one more dimension. The third dimension cannot be chosen arbitrarily, since $[b^p_q]$ must belong to the particular de Sitter group and due to $b^5_5 = 0$ the equation

$$b^5_i g^{ij} b^5_j = g^{55} \tag{5.11}$$

must be satisfied. Thus if the de Sitter group is the type (4,1) (e.g., $g^{55} = +1$), the maximum dimension reduction can be achieved by

$$b^5_1 = b^5_2 = b^5_4 = b^5_5 = 0, \quad b^5_3 = 1 ,$$

while if the type is (3,2) ($g^{55} = -1$) then we have

$$b^5_1 = b^5_2 = b^5_3 = b^5_5 = 0, \quad b^5_4 = 1 .$$

In both cases the minimum dimension is 1, but its character (spatial or temporal) depends on the type of the de Sitter group.

VI. DIMENSION REDUCTION IN SPHERICAL COORDINATES

The maximum reduction described in the previous section is allowed by the ultimate symmetry of the flat space-time expressed in Cartesian coordinates. The gauge transformation is also constant and cannot be continuously changed into the identity. It is of interest to study variable transformations that can reduce the dimension of a finite region of space-time while remaining everywhere continuous. In particular, eliminating the radial distance could lead to a model of a pointlike particle that would at the same time occupy a finite region of the base manifold and thus preserve an inter-

nal structure. This could be used also for dealing with classical singularities caused by pointlike character of particles. The Schwarzschild metric should be investigated in this manner, but here only the reduction of a flat space-time metric in spherical coordinates will be considered as a preliminary study.

In the initial gauge we can choose

$$A^{\,1}_{r} = (1/l)\cos\theta, \quad A^{\,2}_{r} = (1/l)\sin\theta\sin\phi, \quad A^{\,3}_{r} = (1/l)\sin\theta\cos\phi\,, \tag{6.1}$$

and

$$A^{\,ij}_{r} = 0 \quad \text{for all } i,j = 1,\ldots,4\,. \tag{6.2}$$

The same reasoning that lead to Eqs. (5.10) now results in

$$A^{\,i}_{r}b^{\,5}_{5} + g^{ij}(\partial_r b^{\,5}_{j}) = 0, \quad i = 1,2,3\,, \qquad g^{4j}(\partial_r b^{\,5}_{j}) = 0\,, \quad -A^{\,k}_{r}b^{\,5}_{k} + (\partial_r b^{\,5}_{5})g^{55} = 0\,. \tag{6.3}$$

Eliminating $b^{\,5}_{j}$ yields

$$g^{55}(\partial^{\,2}_{r}b^{\,5}_{5}) + (1/l^{\,2})b^{\,5}_{5} = 0\,, \tag{6.4}$$

with the general solution

$$b^{\,5}_{5} = a\cos(r/l) + b\sin(r/l)\,, \tag{6.5}$$

if $g^{55} = +1$ [the case of (4,1) de Sitter group], and

$$b^{\,5}_{5} = ae^{r/l} + be^{-r/l}\,, \tag{6.6}$$

if $g^{55} = -1$ [the case of (3,2) de Sitter group].

For example, a complete solution for the (4,1) case can be written as

$$[b^{\,p}_{q}] = \begin{bmatrix} 0 & \cos\phi & -\sin\phi & 0 & 0 \\ \sin\theta & -\cos\theta\sin\phi & -\cos\theta\cos\phi & 0 & 0 \\ \cos(r/l)\cos\theta & \cos(r/l)\sin\theta\sin\phi & \cos(r/l)\sin\theta\cos\phi & 0 & \sin(r/l) \\ 0 & 0 & 0 & 1 & 0 \\ -\sin(r/l)\cos\theta & -\sin(r/l)\sin\theta\sin\phi & -\sin(r/l)\sin\theta\cos\phi & 0 & \cos(r/l) \end{bmatrix}. \tag{6.7}$$

At $r = 2\pi nl$, n integer, the gauge transformation (6.7) reduces to a 3×3 transformation of spatial frames. The fact that it does not reach the identity is due to the nonexistence of a global frame selection on a spherical surface, and it could be fixed by using an appropriate patching. The important feature is that the translational components of the gauge transformation disappear on the surface of radius $2\pi nl$. Thus it is possible to have a continuous gauge transformation that leaves the outside of the sphere as the four-dimensional space-time, while the inside region loses one observable dimension, namely the radial distance.

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Quantization: Towards a comparison between methods

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In this paper it is shown that the procedure of geometric quantiztion applied to Kähler manifolds gives the following result: the Hilbert space $\mathscr{H}$ consists, roughly speaking, of holomorphic functions on the phase space M and to each classical observable f (i.e., a real function on M) is associated an operator $\mathbf{f}$ on $\mathscr{H}$ as follows: first multiply by $f + \frac{1}{4}\hbar\Delta_{\mathrm{dR}}f$ (Δ_{dR} being the Laplace–de Rham operator on the Kähler manifold M) and then take the holomorphic part [see G. M. Tuynman, J. Math. Phys. **27**, 573 (1987)]. This result is correct on compact Kähler manifolds and correct modulo a boundary term $\int_M d\alpha$ on noncompact Kähler manifolds. In this way these results can be compared with the quantization procedure of Berezin [Math. USSR Izv. **8**, 1109 (1974); **9**, 341 (1975); Commun. Math. Phys. **40**, 153 (1975)], which is strongly related to quantization by *-products [e.g., see C. Moreno and P. Ortega-Navarro; Ann. Inst. H. Poincaré Sec. A: **38**, 215 (1983); Lett. Math. Phys. **7**, 181 (1983); C. Moreno, Lett. Math. Phys. **11**, 361 (1986); **12**, 217 (1986)]. It is shown that on irreducible Hermitian spaces [see S. Helgason, *Differential Geometry, Lie Groups and Symmetric Spaces* (Academic, Orlando, FL, 1978)] the contravariant symbols (in the sense of Berezin) of the operators $\mathbf{f}$ as above are given by the functions $f + \frac{1}{4}\hbar\Delta_{\mathrm{dR}}f$. The difference with the quantization result of Berezin is discussed and a change in the geometric quantization scheme is proposed.

I. PRELIMINARIES

Let (M,ω) be a symplectic manifold describing the phase space of some physical system in classical mechanics. By n we always denote half the (real) dimension of M and by ϵ_k we denote the $2k$-form on M,

$$\epsilon_k = (-1)^{k(k-1)/2}/k!\,\omega^k,$$

in particular, $\epsilon_0 = 1$ and ϵ_n is the Liouville volume element on M. On M we choose the orientation such that ϵ_n is positive and hence we can (and will) identify densities and volume forms on M.

Geometric quantization with the metalinear correction incorporated then constructs a Hilbert space $\mathscr{H}$ out of sections of a complex line bundle QB over M and assigns (tries to assign) to an observable f (i.e., $f: M \to \mathbb{R}$) an operator $\mathbf{f}$ on $\mathscr{H}$. In Ref. 1 a general formula is derived for the local expression of the inner product on $\mathscr{H}$ and moreover, for those observables satisfying $[X_f, P + P^\dagger] \subset P + P^\dagger$ a general (local) expression for $\mathbf{f}$ is given that is derived by means of an infinitesimal pairing (Ref. 2) [X_f denotes the Hamiltonian vector field associated to the function f: $i_{X_f}\omega + df = 0$, P denotes the polarization and † means complex conjugation (*and in case of matrices it means transposition as well*)].

We now briefly recall those formulas, in case the polarization P is a positive Kähler polarization. The prequantum bundle L (see, for instance, Refs. 2 or 3) is constructed by means of a set of local potentials ϑ_j on U_j for ω (i.e., $d\vartheta_j = \omega$), where $\{U_j\}$ covers the symplectic manifold M. On $U_j \cap U_k$ one supposes $\vartheta_j - \vartheta_k = du_{jk}$ for some function u_{jk} and then the transition functions of the bundle L are given by $\exp(iu_{jk}/\hbar)$. In the sequel we will identify local sections of L with functions on M, always with respect to such a trivialization, i.e., depending on the choices of local symplectic potentials ϑ_j. The quantum bundle QB is defined as the tensor product of L with a line bundle associated to the bundle of metalinear P frames. Since the bundle of metalinear P frames has (locally) a canonical trivialization in the case of a Kähler polarization (see Ref. 1), it follows that our trivialization of L defines a trivilization of QB. Let ψ_0 be a local nowhere-zero section of L (i.e., identified with a local nowhere-zero function) that is covariant constant along the polarization P (with respect to the connection ∇ on L, see below) and let $z^1,\ldots,z^n$ be local complex coordinates on M. These coordinates exist because (M,ω) together with a positive Kähler polarization determine a complex structure on M for which ω is a (positive) Kähler form (e.g., see Ref. 4). With ψ_0 and z^j as above each global section ψ of QB which is covariant constant along P determines (uniquely) a local holomorphic function $h(z)$ such that locally $\psi = h\psi_0$. Moreover, $\mathscr{H}$ consists of these covariant constant sections of QB; to two such sections ψ and ψ' is associated a density ≡ measure ≡ volume form (ψ',ψ) on M and the inner product $\langle\psi',\psi\rangle$ in $\mathscr{H}$ is calculated by integration of (ψ',ψ) over M.

Because of the one-to-one relation between sections of QB that are covariant constant in the direction of P and (local) holomorphic functions on M we will use the two notations ψ and h, with $\psi = h\psi_0$ interchangeably. With these conventions the local expression for (ψ',ψ) as given in Ref. 1 becomes

$$(\psi',\psi)(z,z^\dagger) = (h',h)(z,z^\dagger) = H_{h',h}(z,z^\dagger)\epsilon_n,$$
$$H_{h',h}(z,z^\dagger) = h'(z)^\dagger h(z)|\psi_0(z,z^\dagger)|^2 \cdot \sqrt{\det((2\pi i\hbar)^{-1} \times \omega(X_{z^j}, X_{z^k}))_{j,k=1,\ldots,n}}. \quad (1.1)$$

Since (ψ',ψ) and ϵ_n are globally defined densities it follows that $H_{h',h}$ is a globally defined function on M. Then $\mathscr{H}$ con-

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sists of those ψ that are covariant constant in the direction of P and for which $\int_M (\psi,\psi')$ is finite. If we omit the condition that h (and h') should be holomorphic (i.e., if we omit the condition that ψ should be covariant constant in the direction of P) then (1.1) defines a density for each pair of global sections of QB and one can consider the Hilbert space $L^2(M,P)$ of square integrable sections. Then $\mathscr{H}$ is the closed subspace of holomorphic sections of $L^2(M,P)$,

$$\mathscr{H} \equiv L^2(M,P)_{\text{hol}} \subset L^2(M,P), \tag{1.2}$$

and the orthogonal projection π: $L^2(M,P) \to \mathscr{H}$ admits a (local) integral representation (local in the sense that it depends upon the chosen trivialization of QB). Now let f be an observable, then for $h \in \mathscr{H}$ we can define a section $L_f h$ of QB (which need not be covariant constant in the direction of P) by

$$(L_f h)\psi_0 = -i\hbar X_f(h\psi_0) + \left(f - \vartheta(X_f) - \frac{1}{2} i\hbar \sum_{j=1}^{n} a_{jj}\right) h\psi_0 \tag{1.3}$$

or equivalently with our identification of a section $h\psi_0$ with the function h,

$$L_f h = -i\hbar X_f h + \left(f - \vartheta(X_f) - i\hbar X_f \log \psi_0 - \frac{1}{2} i\hbar \sum_j a_{jj}\right) h,$$

where a_{jk} is defined by the equation

$$[X_f, X_{z^j}] = \sum_k (a_{jk} X_{z^k} + b_{jk} X_{z^{k\dagger}})$$

and where ϑ is a local potential for $\omega (d\vartheta = \omega)$, used to define the trivialization of the prequantum bundle L; the combination

$$\nabla_X (h\psi_0) = X(h\psi_0) - (i/\hbar)\vartheta(X)(h\psi_0)$$

is the local expression for the connection ∇ on L acting on the section $h\psi_0$ in the direction X. Using the general Blattner–Kostant–Sternberg (BKS) kernel one can show that the operator $\mathbf{f}$ acting on h as defined by the method of infinitesimal pairing is given by the orthogonal projection of $L_f h$ on $\mathscr{H}$; more precisely,

$$\text{domain } \mathbf{f} = \{h \in \mathscr{H} \mid L_f h \in L^2(M,P)\},$$

and

$$\mathbf{f}h = \pi L_f h \Leftrightarrow \forall h' \in \mathscr{H}\ \forall h \in \text{domain } \mathbf{f}\text{: } \langle h', \mathbf{f}h \rangle = \int_M (h', L_f h). \tag{1.4}$$

II. ON KÄHLER MANIFOLDS

In this section we briefly recall some elementary facts about Kähler manifolds, and then apply them to formulas (1.1) and (1.3). Our basic reference will be the book of Weil[5] and we will adopt the conventions used therein. A Kähler manifold M is a complex manifold with a (complex) Hermitian inner product G on each tangent space: if $z^1,\ldots,z^n$ are local complex coordinates then

$$G(m) = g_{jk}(m) dz^j \otimes dz^{k\dagger} \quad \text{with} \quad g_{jk}^{\dagger} = g_{kj};$$

(g_{jk}) should be positive definite and we denote by g the determinant of (g_{jk}),

$$g = \det(g_{jk}).$$

The imaginary part ω of G, $\omega = \text{Im } G$, is an antisymmetric two-tensor, hence a two-form. In the local coordinates z^j we have

$$\omega = \tfrac{1}{2} i g_{jk} dz^k \wedge dz^{j\dagger},$$

and the condition M is Kähler equivalent to the condition ω symplectic. On the other hand, the real part of G defines a Riemannian structure on M seen as a real manifold (of dimension $2n$) and hence there exists a Laplace–de Rham operator Δ_{dR} on forms. In the local coordinates this operator is expressed on functions f: $M \to \mathbb{R}$ as

$$\Delta_{\text{dR}} f = -4 g^{jk} \cdot \frac{\partial^2 f}{\partial z^j \partial z^{k\dagger}} \quad \text{with} \quad g^{jk} \cdot g_{km} = \delta_m^j. \tag{2.1}$$

The invariant volume form associated to this Riemannian structure is the form ϵ_n; if we denote $z^j = x^j + iy^j$ then

$$\epsilon_n = (\tfrac{1}{2} i)^n \cdot g \cdot dz^1 \wedge \cdots \wedge dz^n \wedge dz^{1\dagger} \wedge \cdots \wedge dz^{n\dagger} = g \cdot dx^1 \wedge \cdots \wedge dx^n \wedge dy^1 \wedge \cdots \wedge dy^n = g \cdot \text{Leb}^{2n}$$

with Leb^n the Lebesgue measure on $\mathbb{R}^n$.

The complex structure on M defines a natural grading of the k-forms and the exterior derivative splits accordingly, $d = d' + d''$ (d' the del operator and d'' the del-bar operator). Using the Grothendieck–Dolbeault lemma on the closed two-form ω of type (1,1) one can show the local existence of a real function F on M such that

$$\omega = \frac{1}{2} i d'd'' F \Leftrightarrow g_{jk} = \frac{\partial^2 F}{\partial z^k \partial z^{j\dagger}}.$$

From this it follows that the local one-form ϑ defined by

$$\vartheta = \frac{1}{4} i(d''F - d'F) = \frac{1}{4} i\left(\frac{\partial F}{\partial z^{k\dagger}} dz^{k\dagger} - \frac{\partial F}{\partial z^k} dz^k\right)$$

is a local symplectic potential. Computing X_{z^j} we find

$$X_{z^j} = -2ig^{jk} \frac{\partial}{\partial z^{k\dagger}}, \quad \vartheta(X_{z^j}) = \frac{1}{4} i X_{z^j} F,$$

$$\omega(X_{z^{j\dagger}}, X_{z^k}) = 2ig^{jk},$$

from which we deduce that the "function" ψ_0 defined by

$$\psi_0 = \exp(-\tfrac{1}{4} F/\hbar)$$

is nowhere vanishing and covariantly constant in the direction of the polarization P spanned by the X_{z^j} [see the definition of ∇ after formula (1.3)]. This polarization is indeed a positive Kähler polarization on M seen as symplectic manifold, and conversely, if P is a positive Kähler polarization on a symplectic manifold then there exist local complex coordinates z^j (turning M into a complex Kähler manifold) such that X_{z^j} span P, a fact that should explain our interest in the local Hamiltonian vector fields X_{z^j}. Finally the condition $d\omega = 0$ implies that

$$\sum_j \left(\frac{\partial g^{jk}}{\partial z^j} + g^{jk} \frac{\partial \log g}{\partial z^j}\right) = 0 \quad (\forall k),$$

and we find after some calculations that the expression $-\frac{1}{2} i\hbar \Sigma_{a_{jj}}$ in (1.3) is given by

$$-\frac{1}{2} \hbar \sum a_{jj} = -\frac{1}{4} \hbar \Delta_{\text{dR}} f - \hbar \frac{\partial \log g}{\partial z^j} \cdot g^{jk} \cdot \frac{\partial f}{\partial z^{k\dagger}}.$$

Combining all these facts and substituting them in (1.1) and (1.3) we find

$$H_{h',h}(z,z^\dagger) = (\pi\hbar)^{-n/2} h'(z)^\dagger h(z) \exp(-\tfrac{1}{2}F/\hbar) g^{-1/2} \tag{2.2}$$

and

$$L_f = -i\hbar X_f h + h\cdot\left[f - \frac{1}{4}\hbar\Delta_{\mathrm{dR}} f - \frac{\partial(F+\hbar\log g)}{\partial z^j}\cdot g^{jk}\cdot\frac{\partial f}{\partial z^{k\dagger}}\right].$$

Since $(h',L_f h)$ figures in the expression for $\mathbf{f}$ we can integrate by parts with respect to X_f inside $(h',L_f h)$ and we find

$$(h',L_f h) = (h',[(1+\tfrac{1}{4}\hbar\Delta_{\mathrm{dR}})f]h) + R_f(h',h), \tag{2.3}$$

$$\begin{aligned} R_f(h',h) &= \sum_{j,k=1}^{n} \frac{\partial}{\partial z^j}\left[(\pi\hbar)^{-n/2} h'(z)^\dagger h(z) \times \exp\left(\frac{-F}{2\hbar}\right) g^{1/2} 2\hbar g^{jk} \frac{\partial f}{\partial z^{k\dagger}}\right] \mathrm{Leb}^{2n} \\ &= (-1)^{n-1} i\hbar\, d'[H_{h',h} d''(f\epsilon_{n-1})] \\ &\equiv (-1)^{n-1} i\hbar\, d[H_{h',h} d''(f\epsilon_{n-1})] = d\alpha. \end{aligned} \tag{2.4}$$

From this expression we see that $\alpha = (-1)^{n-1} \times i\hbar H_{h',h} d''(f\epsilon_{n-1})$ is a well-defined global $(2n-1)$-form on M (because $H_{h',h}$, f and ϵ_{n-1} are global), so $R_f(h',h)$ is an exact $2n$-form and the following theorem immediately follows.

Theorem 2.1: If M is a compact Kähler manifold without boundary, if $f: M \to \mathbb{R}$ is any observable, and if ψ, $\psi' \in \mathscr{H}$ are global sections of QB, then

$$\mathbf{f}\psi = \pi([(1+\tfrac{1}{4}\hbar\Delta_{\mathrm{dR}})f]\psi) \quad \text{(orthogonal projection)},$$

or equivalently

$$\langle\psi',\mathbf{f}\psi\rangle = \int_M \left(\psi',\left[\left(1+\frac{1}{4}\hbar\Delta_{\mathrm{dR}}\right)f\right]\psi\right).$$

Remark 2.2: If M is not compact then there might be an extra term resulting from $\int_M d\alpha$, which depends on the behavior of α "at infinity" (or at the "boundary" of M). In Secs. IV and V we will consider the cases $M = \mathbb{C}$ and M is an irreducible Hermitian symmetric space of noncompact type and in these cases we will redefine $\mathbf{f}$ as if Theorem 2.1 were true for these noncompact spaces. We then will give some examples to make plausible that the boundary term $\int d\alpha$ is 0 for physically interesting observables, which should justify the redefinition of $\mathbf{f}$.

Remark 2.3: There is a remarkable resemblance between $R_f(h',h)$ and the inner product (h',h):

$$(h',h) = H_{h',h}\epsilon_n = (-1)^{n-1} i(2n)^{-1} H_{h',h} d\, d''(F\epsilon_{n-1}),$$

$$R_f(h',h) = d[(-1)^{n-1} i\hbar H_{h',h} d''(f\epsilon_{n-1})].$$

III. INTERMEZZO

In this (brief) section we recall some definitions of Berezin[6,7] in order to be able to compare our results with his. Let $\mathscr{H}$ be a Hilbert space and M^0 a manifold with measure μ and let $E = \{e_m \mid m \in M^0\}$ be a set of vectors in $\mathscr{H}$.

Definition 3.1: The system E is called (super) complete iff

$$\forall f,g \in \mathscr{H}: \quad \langle f,g\rangle = \int_{M^0} \langle f,e_m\rangle\langle e_m,g\rangle d\mu(m).$$

It follows that $\mathscr{H}$ can be embedded in $L^2(M^0,\mu)$ by $f \in \mathscr{H} \to f(m) = \langle e_m, f\rangle$.

Definition 3.2: Suppose E is a super complete system and $\mathbf{A}$ is an operator such that E is contained in the domain of $\mathbf{A}$, then the function A_0 defined by

$$A_0(m) = \langle e_m, \mathbf{A}e_m\rangle / \langle e_m, e_m\rangle$$

is called the *covariant symbol* of the operator $\mathbf{A}$.

Definition 3.3: Let E be a super complete system and $\mathbf{A}$ an operator that can be calculated by

$$\langle f,\mathbf{A}g\rangle = \int_{M^0} \langle f,e_m\rangle A^0(m)\langle e_m,g\rangle d\mu(m)$$

for some function A^0 on M^0, then A^0 is called the *contravariant symbol* of the operator $\mathbf{A}$.

Proposition 3.4: Suppose $\mathbf{A}$ is an operator on $\mathscr{H}$ for which both the covariant and contravariant symbol exist, then we have

$$A_0(m') = \int_{M_0} \frac{\langle e_{m'},e_m\rangle\langle e_m,e_{m'}\rangle}{\langle e_{m'},e_{m'}\rangle} A^0(m) d\mu(m).$$

IV. QUANTIZATION ON $\mathbb{C}$

On $M = \mathbb{C}$ with complex coordinate $z = x + iy$ we use the symplectic form $\omega = \frac{1}{2}\lambda\, dz \wedge dz^\dagger = \lambda\, dx \wedge dy$. For $\lambda > 0$ the polarization $P = \mathbb{C}X_z$ is a positive Kähler polarization, so we can apply the theory of Secs. I and II. The global function $F = \lambda zz^\dagger$ satisfies $\omega = \frac{1}{2}id'd''F$ so the general (local) formulas (1.1), (1.2), (2.1), (2.2), and (2.4) become global and reduce to

$$L^2(\mathbb{C},P) = \left\{h: \mathbb{C}\to\mathbb{C} \,\middle|\, \int_{\mathbb{C}} |h(z)|^2 \times \exp\left(\frac{-\lambda zz^\dagger}{2\hbar}\right) d\,\mathrm{Leb}^2 < \infty\right\},$$

$$\mathscr{H} = \{h \in L^2(\mathbb{C},P) \mid h \text{ is holomorphic}\},$$

$$\langle h',h\rangle = \pi^{-1/2}\left(\frac{\lambda}{\hbar}\right)^{1/2} \int_{\mathbb{C}} h'(z)^\dagger h(z) \times \exp\left(\frac{-\lambda zz^\dagger}{2\hbar}\right) d\,\mathrm{Leb}^2,$$

$$\Delta_{\mathrm{dR}} = -4\lambda^{-1}\frac{\partial^2}{\partial z\,\partial z^\dagger} = -\lambda^{-1}(\partial_x^2 + \partial_y^2),$$

$$R_f(h',h) = d[i\pi^{-1/2}(\hbar/\lambda)^{1/2} h'(z)^\dagger h(z) \times \exp(-\tfrac{1}{2}\lambda zz^\dagger/\hbar) d''f].$$

Remark 4.1: In physics a symplectic form has the same units as an angular momentum $[\mathrm{kg\,m^2\,sec^{-1}}] \equiv [\mathrm{Joule\ sec}]$; in mathematics coordinates usually do not have any units, so one expects the symplectic form to have no units. In order to separate these two aspects of a symplectic form we have introduced a parameter λ which has the same units as

Planck's constant $\hbar$ (i.e., Joule sec) and we have introduced dimensionless coordinates $z = x + iy$; all units have been absorbed in the parameter λ. As is clear from the above formulas, in relevant formulas this parameter always occurs in the combination $\lambda/\hbar$, which is dimensionless (the combination $\hbar\Delta_{\mathrm{dR}}$ is dimensionless and it is this combination that occurs in the expression for the operators), so one might be tempted to omit one of them (as does Berezin, see Ref. 6). We will not do so, because λ and $\hbar$ have different physical interpretations: λ represents a physical quantity and $\hbar$ represents the quantum mechanical yard stick with which to measure λ. In Secs. V and VI a parameter λ will be introduced in the same way as in this section and with the same motivations; in this section one can imagine that λ represents the mass of the (one-dimensional) system, in case $M = S^2 (= M^I_{1,1}$, see Sec. VI) λ represents the intrinsic angular momentum (spin) (see for instance Refs. 8 and 9).

For an observable f we now define (redefine) (the domain of) $\mathfrak{f}$ as follows:

$$\text{domain } \mathfrak{f} = \{h \in \mathscr{H} \mid [(1 + \tfrac{1}{4}\hbar\Delta_{\mathrm{dR}})f]h \in L^2(\mathbb{C},P)\},$$

$$\mathfrak{f}h = \pi([1 + \tfrac{1}{4}\hbar\Delta_{\mathrm{dR}})f]h)$$

$$= \pi([f - \tfrac{1}{4}(\hbar/\lambda)(\partial_x^2 + \partial_y^2)f]h).$$

This definition is different from the definition given in Sec. I, but we will make plausible by means of examples that in interesting cases if $h \in$ domain $\mathfrak{f}$ and $h' \in \mathscr{H}$ then $\int R_f(h',h) = 0$, which implies that then the two definitions "coincide," the only possible difference being the case that in (2.3) the left-hand side $(h', L_f h)$ is finite whereas both terms on the right-hand side are infinite.

Proposition 4.2: If $\partial f/\partial z^\dagger$ is bounded on $\mathbb{C}$ then $\int_{\mathbb{C}} R_f(h',h) = 0$ for all $h', h \in \mathscr{H}$.

Proof: For $h', h \in \mathscr{H}$ the function $G = \pi^{-1/2} \times (\lambda/\hbar)^{1/2} h'(z)^\dagger h(z) \exp(-\frac{1}{2}\lambda z z^\dagger \hbar)$ is absolutely integrable over $\mathbb{C}$ (it is the integrand of $\langle h', h\rangle$) so

$$\int_{\mathbb{C}} |G| d\,\mathrm{Leb}^2 = \int_0^\infty dR \int_0^{2\pi} d\varphi\, R\,|G| < \infty,$$

hence there exists a sequence R_k tending to ∞ such that

$$\lim_{k\to\infty} \int_{|z| = R_k} R_k |G| d\varphi = 0.$$

We now have

$$|R_f(h',h)| = \left| \lim_{k\to\infty} \int_{|z|<R_k} d[G, d''f] \right|$$

$$= \lim_{k\to\infty} \left| \int_{|z| = R_k} G d''f \right|$$

$$\leqslant \lim_{k\to\infty} \int_{|z| = R_k} |G| R_k \left| \frac{\partial f}{\partial z^\dagger} \right| d\varphi$$

$$\leqslant \text{const} \lim_{k\to\infty} \int_0^{2\pi} |G| R_k\, d\varphi = 0,$$

where the last inequality is a consequence of our assumption. Q.E.D.

Proposition 4.3: If $|\partial f/\partial z^\dagger| \leqslant c_1 |(1 + \frac{1}{4}\hbar\Delta_{\mathrm{dR}})f| + c_2$ for some positive constants c_1 and c_2 then $h \in$ domain $\mathfrak{f}$ and $h' \in \mathscr{H} \Rightarrow \int_{\mathbb{C}} R_f(h',h) = 0$.

Proof: If we define G as in Proposition 4.2 then the conditions show that the function $c_1|[(1 + \frac{1}{4}\hbar\Delta_{\mathrm{dR}})f]G| + c_2|G|$ has a finite integral over $\mathbb{C}$ and then we can apply the same reasoning as in Proposition 4.2. Q.E.D.

Remark 4.4: Proposition 4.2 is clearly a special case of Proposition 4.3, although the statement is slightly stronger. The condition mentioned in Proposition 4.3 is true for the observables x, y (linear momentum and position), x^2, y^2, and $x^2 + y^2$ (kinetic energy, quadratic potential, and the harmonic oscillator) so for these observables both definitions coincide, i.e., for these observables the procedure of geometric quantization gives the result of Theorem 2.1 for the (noncompact) manifold $\mathbb{C}$.

Remark 4.5: The condition of Proposition 4.3 is not satisfied by $f = xy = z^2 - z^{\dagger 2}$. However, if we are interested in the angular momentum, then we have to consider the symplectic manifold $\mathbb{C}^n (n > 1)$ and there one can show with the same arguments that for $f = x_1 y_2 - x_2 y_1 = z_1 z_2^\dagger - z_2 z_1^\dagger$ then again the two definitions coincide.

We now turn our attention to the orthogonal projection $\pi: L^2(\mathbb{C},P) \to \mathscr{H}$; it is well known that π admits an integral representation with a Bergman kernel $K_\lambda(w,z^\dagger)$ defined by

$$K_\lambda(w,z^\dagger) = \frac{1}{2}\pi^{-1/2}\left(\frac{\lambda}{\hbar}\right)^{1/2} \exp\left(\frac{\lambda w z^\dagger}{2\hbar}\right)$$

and

$$(\pi g)(w) = \pi^{-1/2}\left(\frac{\lambda}{\hbar}\right)^{1/2} \int_{\mathbb{C}} K_\lambda(w,z^\dagger) g(z,z^\dagger)$$

$$\times \exp\left(\frac{-\lambda z z^\dagger}{2\hbar}\right) d\,\mathrm{Leb}^2(z).$$

If we define the elements $e_w \in \mathscr{H}$ by $e_w(z) = K_\lambda(z,w^\dagger)$ then this becomes

$$(\pi g)(w) = \langle e_w, g\rangle \quad [\text{inner product in } L^2(\mathbb{C},P)].$$

Since π is a projection we have the reproducing property formula for $g \in \mathscr{H}$: $g(w) = \langle e_w, g\rangle$, whence the set $\{e_w \mid w \in \mathbb{C}\}$ is a supercomplete system in the sense of Berezin if we denote by μ the measure defined by

$$d\mu(z) = \pi^{-1/2}(\lambda/\hbar)^{1/2} \exp(-\tfrac{1}{2}\lambda z z^\dagger/\hbar) d\,\mathrm{Leb}^2(z).$$

With these conventions the expression for $\mathfrak{f}$ becomes

$$\langle h', \mathfrak{f}h\rangle = \int h'(z)^\dagger \left[\left\{1 + \frac{1}{4}\hbar\Delta_{\mathrm{dR}}\right\} f\right] h(z) d\mu(z)$$

$$= \int \langle h', e_z\rangle \left[\left(1 + \frac{1}{4}\hbar\Delta_{\mathrm{dR}}\right) f\right] \langle e_z, h\rangle d\mu(z),$$

so the contravariant symbol of $\mathfrak{f}$ is the function

$$\mathrm{contravar}(\mathfrak{f}) = (1 + \tfrac{1}{4}\hbar\Delta_{\mathrm{dR}})f.$$

For $M = \mathbb{C}$ the relation between covariant and contravariant symbols is known (see Ref. 6),

$$A_0 = \exp(-\tfrac{1}{2}\hbar\Delta_{\mathrm{dR}})A^0,$$

from which we deduce

$$\mathrm{covar}(\mathfrak{f}) = (1 + \tfrac{1}{4}\hbar\Delta_{\mathrm{dR}})\exp(-\tfrac{1}{2}\hbar\Delta_{\mathrm{dR}})f. \qquad (4.1)$$

V. QUANTIZATION ON IRREDUCIBLE HERMITIAN SYMMETRIC SPACES OF NONCOMPACT TYPE

According to the general theory[10] the four series of irreducible noncompact Hermitian symmetric spaces are just the classical bounded domains in $\mathbb{C}^n$ (Ref. 11). These domains are characterized by matrices as described in Table I (matrix $A>0$ means all eigenvalues positive). In the sequel we will often identify a set of coordinates $(z^1,\ldots,z^n)$ with the corresponding matrix, so depending on the context z means either the matrix or the set of coordinates.

These four series can also be described as certain homogeneous spaces; this alternative description is listed in Table II. When seen as bounded domains, these spaces possess a (classical) Bergman kernel $K(z,w^\dagger)$ (see Ref. 11) that is also listed in Table II (up to a multiplicative constant). We now introduce a Kähler structure on Ω (for all four series simultaneously) by

$$\omega = \tfrac{1}{2}id'd''F \quad \text{with} \quad F(z,z^\dagger) = \lambda \log K(z,z^\dagger)$$

for λ positive and real.

The associated (positive definite) Hermitian metric is (apart from a multiplicative constant) the usual Bergman metric which is invariant under the holomorphic diffeomorphisms of Ω. Since each Ω is homogeneous (the group G can be realized as holomorphic isometries of Ω) there exist positive constants $c(\Omega)$ such that

$$g = \det\left(\frac{\partial^2 F}{\partial z\,\partial z^\dagger}\right) = c(\Omega)\lambda^n K(z,z^\dagger).$$

Finally, the polarization P spanned by (X_{z^j}) is a positive Kähler polarization with respect to the symplectic form ω defined above and, moreover, F is global so the (local) formula (1.1), (1.2), (2.2), and (2.4) are global:

$$L^2(\Omega,P) = \left\{h:\Omega\to\mathbb{C}\,\middle|\,\int_\Omega |h(z)|^2 K(z,z^\dagger)^{1-\lambda/\hbar/2}\,d\,\mathrm{Leb}^{2n} < \infty\right\}, \quad \mathscr{H} = \{h\in L^2(\Omega,P)\,|\,h \text{ is holomorphic}\},$$

$$\langle h',h\rangle = c(\Omega)^{-1/2}(\pi\lambda\hbar)^{-n/2}\int_\Omega h'(z)^\dagger h(z) K(z,z^\dagger)^{-(1+\lambda/\hbar)/2}\epsilon_n$$

$$= c(\Omega)^{1/2}\pi^{-n/2}(\lambda/\hbar)^{n/2}\int_\Omega h'(z)^\dagger h(z) K(z,z^\dagger)^{(1-\lambda/\hbar)/2}\,d\,\mathrm{Leb}^{2n},$$

$$R_f(h',h) = d\left[(-1)^{n-1} i\hbar\, c(\Omega)^{-1/2}(\pi\lambda\hbar)^{-n/2} h'(z)^\dagger h(z) K(z,z^\dagger)^{-(1+\lambda/\hbar)/2}\, d''(f\epsilon_{n-1})\right].$$

Remark 5.1: For $\lambda/\hbar = 1$ we see that $\mathscr{H}$ is the ordinary Hilbert space of holomorphic, square integrable functions on the domain Ω (with respect to the Lebesgue measure). For more comments on the interpretation of the parameter λ, see Remark 4.1.

Remark 5.2: In Ref. 12 Berezin introduces a parameter h^{-1} when quantizing irreducible Hermitian symmetric spaces of noncompact type, a parameter which in our treatment is given by $\frac{1}{2}(1+\lambda/\hbar)$ (see also Remark 4.1). After the introduction of h^{-1} he gives a definition of "allowed value" for h^{-1} that is, roughly speaking, the following condition: the Hilbert space $\mathscr{H}$ depends upon the parameter h^{-1} (i.e., on λ) and h_0^{-1} is allowed if $\mathscr{H}(h^{-1})$ is "analytic" in a neighborhood of h_0^{-1}. He then shows that the set of allowed values consists of a continuous part and a discrete part. In our case with $\lambda>0$ the corresponding value of h^{-1} always lies in the continuous part, i.e., in the set of allowed values.

For irreducible Hermitian symmetric spaces of compact type there is in Ref. 12 also a parameter h^{-1} and a definition of allowed value, but in the compact case the definition of allowed value is different from the noncompact case (see for more details Sec. VI after Theorem 6.5).

As on $\mathbb{C}$ we now define (redefine) for an observable f: $\Omega\to\mathbb{R}$ (the domain of) the operator f as follows:

$$\text{domain f} = \left\{h\in\mathscr{H}\,\middle|\,h\left(1+\frac{1}{4}\hbar\Delta_{\mathrm{dR}}\right)f\in L^2(\Omega,P)\wedge\forall h'\in\mathscr{H}:\int_\Omega R_f(h',h)=0\right\}, \quad \mathrm{f}h = \pi\left(\left[\left(1+\tfrac{1}{4}\hbar\Delta_{\mathrm{dR}}\right)f\right]h\right),$$

and again we wish to make plausible that this definition does not differ very much from the definition given in Sec. I. We do this by considering the case $\Omega^{\mathrm{I}}_{1,1}$, which can be interpreted as the Lobatschevsky plane $\cong\Omega^{\mathrm{I}}_{1,1} = D^1 = \{z\in\mathbb{C}\,|\,|z|<1\}$.

Proposition 5.3: If f: $D^1\to\mathbb{R}$ is such that $\partial f/\partial z^\dagger$ is bounded by $(1-zz^\dagger)^{-1}$ on D^1 then $\int_{D^1} R_f(h',h)=0$ for all $h',h\in\mathscr{H}$.

Proof: On D^1 we have $K(z,z^\dagger) = (1-zz^\dagger)^{-2}$ so assuming $h',h\in\mathscr{H}$ we find

TABLE I. Irreducible Hermitian symmetric spaces of noncompact type.

Name	Description	Coordinates	Condition	$n\equiv\mathbb{C}$ dimension
$\Omega^{\mathrm{I}}_{p,q}$	matrices z of order $p\times q$	all pq entries of z	$I-zz^\dagger>0$	$p\cdot q$
Ω^{II}_{p}	symmetric matrices z of order $p\times p$	the upper triangle including the diagonal	$I-zz^\dagger>0$	$\frac{1}{2}p(p+1)$
$\Omega^{\mathrm{III}}_{p}$	antisymmetric matrices z of order $p\times p$	the upper triangle without the diagonal	$I-zz^\dagger>0$	$\frac{1}{2}p(p-1)$
Ω^{IV}_{p}	row vectors z in $\mathbb{C}^p$	all p entries	$\begin{cases}1+\lvert zz^T\rvert^2-2zz^\dagger>0\\ \lvert zz^T\rvert<1\ (^T=\text{transpose})\end{cases}$	p

$$\int_{D^1} |h'(z)^\dagger h(z) K(z,z^\dagger)^{-(1+\lambda/\hbar)/2} K(z,z^\dagger)| d\,\mathrm{Leb}^2 < \infty$$

$$\Leftrightarrow \int_0^1 (1-R^2)^{-1}\, dR \int_0^{2\pi} |h'(z)^\dagger h(z)| (1-R^2)^{\lambda/\hbar} R\, d\varphi < \infty$$

$$\Rightarrow \exists R_k \uparrow 1 \colon \lim_{k\to\infty} \int_0^{2\pi} |h'(z)^\dagger h(z)| (1-R_k^2)^{\lambda/\hbar} R_k\, d\varphi = 0$$

$$\Rightarrow \left| \int_{D^1} R_f(h',h) \right| \leqslant \lim_{k\to\infty} \int_{|z|=R_k} |h'^\dagger h\, | \mathrm{const} (1-R_k^2)^{1+\lambda/\hbar} \left| \frac{\partial f}{\partial z^\dagger}\, dz^\dagger \right|$$

$$\leqslant \lim_{k\to\infty} \mathrm{const} \int_0^{2\pi} |h'(z)^\dagger h(z)| (1-R_k^2)^{\lambda/\hbar} R_k\, d\varphi = 0. \qquad \text{Q.E.D.}$$

Proposition 5.4: Let f: $D^1 \to \mathbf{R}$ and suppose there exist positive constants c_1 and c_2 such that $(1-zz^\dagger)|\partial f \partial z^\dagger| \leqslant c_1 |(1+\frac{1}{4}\hbar\Delta_{\mathrm{dR}})f| + c_2$ on D^1 then $h \in$ domain $\mathbf{f}$ and $h' \in \mathscr{H} \Rightarrow \int R_f(h',h) = 0$.

Proof: If one pastes together the arguments of the proofs of Proposition 4.3 and 5.3 then one obtains easily a proof for this proposition. Q.E.D.

Example 5.5: The group SU(1,1) acts on D^1 as the group of holomorphic symplectic isometries by

$$g = \begin{pmatrix} a & b \\ b^\dagger & a^\dagger \end{pmatrix} \colon \quad z \to \frac{az+b}{b^\dagger z + a^\dagger},$$

$$g \in \mathrm{SU}(1,1) \Leftrightarrow |a|^2 - |b|^2 = 1.$$

We can exhibit three one-parameter subgroups $g_j(t)$ of SU(1,1),

$$g_1(t) = \begin{pmatrix} \cosh t & \sinh t \\ \sinh t & \cosh t \end{pmatrix},$$

$$g_2(t) = \begin{pmatrix} \cosh t & i \sinh t \\ -i \sinh t & \cosh t \end{pmatrix}, \quad g_3(t) = \begin{pmatrix} e^{it} & 0 \\ 0 & e^{-it} \end{pmatrix},$$

which become after differentiation the generators of the Lie algebra su(1,1):

$$g_1'(0) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad g_2'(0) = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix},$$

$$g_3'(0) = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}.$$

The momentum map[8,13,14] associated to this action maps these three generators of the Lie algebra to the functions:

$$f_1 = -i\lambda \frac{z^\dagger - z}{1-zz^\dagger}, \quad f_2 = \lambda \frac{z^\dagger + z}{1-zz^\dagger}, \quad f_3 = \lambda \frac{1+zz^\dagger}{1-zz^\dagger}.$$

TABLE II. Bergman kernels for the bounded domains.

Name	$K(z,w^\dagger)$	Alternative description as G/K (see Ref. 10)
$\Omega_{p,q}^{\mathrm{I}}$	$\det(\mathbf{1}_p - zw^\dagger)^{-p-q}$	$\mathrm{SU}(p,q)/S(U(p)\times U(q))$
Ω_p^{II}	$\det(\mathbf{1}_p - zw^\dagger)^{-p-1}$	$\mathrm{Sp}(p,\mathbf{R})/\mathrm{U}(p)$
Ω_p^{III}	$\det(\mathbf{1}_p - zw^\dagger)^{-p+1}$	$\mathrm{SO}^*(2p)/\mathrm{U}(p)$
Ω_p^{IV}	$(1-2zw^\dagger + zz^T(ww^T)^\dagger)^{-p}$	$\mathrm{SO}_0(p,2)/(\mathrm{SO}(p)\times\mathrm{SO}(2))$

One can show that these functions satisfy the condition of Proposition 5.4, so in computing $\mathbf{f}_j$ we can forget about the term $R_f(h',h)$. Since SU(1,1) acts holomorphically, the associated Hamiltonian vector fields X_{f_j} leave the polarization P invariant, which shows that $L_f h$ is already in $\mathscr{H}$ and we find

$$(L_{f_1} h)(z) = (\mathbf{f}_1) h(z)$$

$$= i\hbar \left((1-z^2)\frac{dh}{dz} - \left(1 + \frac{\lambda}{\hbar}\right) z h(z) \right)$$

$$= \pi(h\,(\mathbf{1} + \tfrac{1}{4}\hbar\Delta_{\mathrm{dR}})f),$$

$$(L_{f_2} h)(z) = (\mathbf{f}_2 h)(z)$$

$$= -\hbar \left((1+z^2)\frac{dh}{dz} + \left(1 + \frac{\lambda}{\hbar}\right) z h(z) \right)$$

$$= \pi(h\,(\mathbf{1} + \tfrac{1}{4}\hbar\Delta_{\mathrm{dR}})f),$$

$$(L_{f_3} h)(z) = (\mathbf{f}_3 h)(z)$$

$$= -\hbar \left(2z\frac{dh}{dz} + \left(1 + \frac{\lambda}{\hbar}\right) z h(z) \right)$$

$$= \pi(h\,(\mathbf{1} + \tfrac{1}{4}\hbar\Delta_{\mathrm{dR}})f).$$

On the other hand, one verifies easily that the action $\rho(g)$ of SU(1,1) on $\mathscr{H}$ given by

$$(\rho(g)h)(z) = (a - b^\dagger z)^{-(1+\lambda/\hbar)} h(g^{-1}z),$$

$g \in \mathrm{SU}(1,1)$ as above,

is a projective representation of SU(1,1) on $\mathscr{H}$. For fixed $g \in \mathrm{SU}(1,1)$ and $|z| < 1$ we have $|a - b^\dagger z| > 0$, so $(a - b^\dagger z)^{-(1+\lambda/\hbar)}$ is holomorphic on D^1; however, such a branch cannot be chosen consistently for all $g \in \mathrm{SU}(1,1)$ simultaneously (see also Ref. 15). For the one-parameter groups $\rho(g_j(t))$ a consistent choice can be made, resulting in a unitary representation of $\mathbf{R}$ on $\mathscr{H}$, showing that their generators $\mathbf{f}_j$ are (essentially) self-adjoint operators:

$$\rho(g_j(t)) = \exp(-it\mathbf{f}_j/\hbar).$$

Back to the general case, the (generalized) Bergman kernel $K_\lambda(z,w^\dagger)$ associated with the orthogonal projection π: $L^2(\Omega,P) \to \mathscr{H}$ is calculated by Berezin,[12]

$$K_\lambda(z,w^\dagger) = \tilde{n}_\lambda(\Omega) K(z,w^\dagger)^{(1+\lambda/\hbar)/2},$$

i.e.,

$$(\pi g)(w) = c(\Omega)^{-1/2}(\pi\lambda\hbar)^{-n/2} \times \int_\Omega K_\lambda(w,z^\dagger) g(z,z^\dagger) K(z,z^\dagger)^{-(1+\lambda/\hbar)/2} \epsilon_n$$
$$= c(\Omega)^{-1/2}(\pi\lambda\hbar)^{-n/2} \tilde{n}_\lambda(\Omega) \times \int_\Omega g(z,z^\dagger) \left[\frac{K(w,z^\dagger)}{K(z,z^\dagger)}\right]^{-(1+\lambda/\hbar)/2} \epsilon_n,$$

where the branch of the mapping $\zeta \to \zeta^{(1+\lambda/\hbar)/2}$ is chosen such that $K_\lambda(z,w^\dagger)$ is real for $z = w$, and the constant $\tilde{n}_\lambda(\Omega)$ is determined by $\tilde{n}_\lambda(\Omega) = \|1\|^{-2}$, where $\|1\|$ denotes the norm in $\mathscr{H}$ of the function which is constant 1 on Ω (it should be noted that indeed $1 \in \mathscr{H}$ for each $\lambda > 0$). If we now define for each $w \in \Omega$ the function $e_w \in \mathscr{H}$ by

$$e_w(z) = K_\lambda(z,w^\dagger),$$

then because of the reproducing property of the orthogonal projection we know that the set $\{e_w | w \in \Omega\}$ is a supercomplete system of elements of $\mathscr{H}$ and, moreover, by definition of domain f, we can show with the same reasoning as in Sec. IV,

$$\text{contravar}(\mathbf{f}) = (1 + \tfrac{1}{4}\hbar\Delta_{\text{dR}})f.$$

The relation between covariant and contravariant symbols is in these cases more complicated then for $M = \mathbb{C}$; explicit expressions for the connecting operator in terms of powers of Δ_{dR} is given by Moreno.[16-18]

VI. QUANTIZATION ON IRREDUCIBLE HERMITIAN SYMMETRIC SPACES OF COMPACT TYPE

In this section the main problem is not to "show" that $R_f(h',h)$ does not contribute to f, because that is guaranteed by compactness, but to exhibit a supercomplete system of vectors in $\mathscr{H}$. In particular, we will show that the allowed values of the parameter h^{-1} of Berezin in Ref. 12 (see Remark 5.2) correspond exactly to the (pre)quantizable values of our parameter λ (quantizable in the sense of Kostant and Souriau, a condition on the cohomology class of the symplectic form).

The four series of irreducible Hermitian symmetric spaces of compact type (which are dual to the noncompact ones) are listed in Table III. As in the noncompact case z denotes either the local coordinates $(z^1,\ldots,z^n)$ or the corresponding matrix. To obtain a full set of local charts we need a (partial) action of G on the local coordinates; therefore we represent each $g \in G$ as block matrices g_{ij} $(i,j = 1,2)$ of appropriate sizes as follows:

$$\begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix} = A(M) g A(M)^{-1},$$

with

$$A(M^{\text{I}}_{p,q}) = \mathbf{1}_{p+q}, \quad A(M^{\text{II}}_p) = \mathbf{1}_{2p},$$
$$A(M^{\text{II}}_p) = \begin{pmatrix} \mathbf{1}_p & i\mathbf{1}_p \\ i\mathbf{1}_p & \mathbf{1}_p \end{pmatrix}, \quad A(M^{\text{IV}}_p) = \begin{pmatrix} \mathbf{1}_p & 0 \\ 0 & i\mathbf{1}_2 \end{pmatrix}$$

(note that as a result each matrix g_{ij} is a special unitary matrix). Using these block matrices one defines the action of G on the local coordinates by

$$gz = (g_{11}z + g_{12})(g_{21}z + g_{22})^{-1}, \quad \text{for types I, II, and III}$$

and

$$gz = \frac{g_{11}z + g_{12}v_z}{(1,i)[g_{21}z + g_{22}v_z]} \quad \text{for type IV,}$$

where v_z is given by $v_z = (\frac{1}{2}(z^Tz + 1), \frac{1}{2}i(z^Tz - 1))^T$. Since the stabilizer of $0 \in \mathbb{C}^n$ is just the subgroup K in the definition of the homogeneous space G/K (Table III) we can use this action of G on $\mathbb{C}^n$ to define a set of local charts $\{U_g | g \in G\}$ for G/K; the chart $\varphi_g: U_g \to \mathbb{C}^n$ is defined by

$$\left.\begin{aligned} &U_g = \{[h] \in G/K \,|\, \det((gh)_{22}) \neq 0\} \\ &\varphi_g: U_g \to \mathbb{C}^n, \quad [h] \to gh(0) = (gh)_{12}(gh)_{22}^{-1} \end{aligned}\right\} \text{for type I, II, and III,}$$

$$\left.\begin{aligned} &U_g = \{[h] \in G/K \,|\, (1,i)(gh)_{22}(1,-i)^T \neq 0\} \\ &\varphi_g: U_g \to \mathbb{C}^n, \quad [h] \to gh(0) = (gh)_{12}(1,-i)^T/(1,i)(gh)_{22}(1,-i)^T \end{aligned}\right\} \text{for type IV,}$$

a chart which covers G/K except for a submanifold of lower dimension. The local diffeomorphisms between two charts U_g and $U_{g'}$ is given by $z \to kz$ for some $k \in G$, more precisely,

$$\varphi_{g'} \circ (\varphi_g)^{-1}: z \to (g'g^{-1})(z). \tag{6.1}$$

On each $M = G/K$ there exists a Kähler structure ω (invariant with respect to the action of G) which is given in local coordinates z by $\omega = \frac{1}{2}id'd''F(z,z^\dagger)$, where F is defined by

$$\left.\begin{aligned} &F(z,z^\dagger) = -\lambda \log K(z,z^\dagger), \quad \lambda > 0, \\ &K(z,w^\dagger) = N(z,w^\dagger)^{-\nu(M)}. \end{aligned}\right. \tag{6.2}$$

The defining functions $N(z,w^\dagger)$ and $\nu(M)$ are given by

TABLE III. Irreducible Hermitian symmetric spaces of compact type.

Name	Description as G/K	Local coordinates	$n \equiv \mathbb{C}$ dimension
$M^{\text{I}}_{p,q}$	$\text{SU}(p+q)/\text{S}(\text{U}(p)\times\text{U}(q))$	matrices z of order $p\times q$	$p\cdot q$
M^{II}_p	$\text{Sp}(p)/\text{U}(p)$	symmetric matrices z of order $p\times p$	$\frac{1}{2}p(p+1)$
M^{III}_p	$\text{SO}(2p)/\text{U}(p)$	antisymmetric matrices z of order $p\times p$	$\frac{1}{2}p(p-1)$
M^{IV}_p	$\text{SO}(p+2)/(\text{SO}(p)\times\text{SO}(2))$	vectors z of length p	p

$$N(z,w^\dagger)=\begin{cases}\det(\mathbf{1}+zw^\dagger), & \text{for types I, II, and III,}\\ 1+2z^Tz+(z^Tz)(z^Tz)^\dagger, & \text{for type IV,}\end{cases} \tag{6.3}$$

$$\begin{aligned}&\nu(M^{\mathrm{I}}_{p,q})=p+q, \quad \nu(M^{\mathrm{III}}_{p})=p-1,\\ &\nu(M^{\mathrm{II}}_{p})=p+1, \quad \nu(M^{\mathrm{IV}}_{p})=p.\end{aligned} \tag{6.4}$$

Since $\lambda>0$ the associated Hermitian metric is positive definite and the polarization P spanned by (X_{z^j}) is a positive Kähler polarization, so again we can apply the general formalism of Sec. II. Since M is homogeneous there exist constants $c(M)$ such that

$$\det\left(\frac{\partial^2 F}{\partial z\,\partial z^\dagger}\right)=c(M)\lambda^n K(z,z^\dagger) \tag{6.5}$$

(here we omit the letter g for this determinant to avoid confusion with the elements of the group G); furthermore, since each local chart U_g covers M except for a set of measure 0 (with respect to ϵ_n = the Liouville measure) it follows that instead of integrating over M we may restrict the integration to the local chart $\mathrm{U_{id}}\cong\mathbb{C}^n$. Hence formulas (1.1), (1.2), and (2.2) become

$$\begin{aligned}L^2(M,P)=\Big\{&h:\mathbb{C}^n\to\mathbb{C}\,|\,h \text{ represents a global section of QB}\\ &\text{and } \int_{\mathbb{C}^n}|h(z)|^2K(z,z^\dagger)^{(\lambda/\hbar+1)/2}\\ &\times d\,\mathrm{Leb}^{2n}<\infty\Big\},\end{aligned}$$

$$\mathscr{H}=\{h\in L^2(M,P)\,|\,h \text{ holomorphic}\},$$

$$\begin{aligned}\langle h',h\rangle&=c(M)^{-1/2}(\pi\lambda\hbar)^{-n/2}\\ &\times\int_{\mathbb{C}^n}h'(z)^\dagger h(z)K(z,z^\dagger)^{(\lambda/\hbar-1)/2}\epsilon_n \qquad (6.6)\\ &=c(M)^{1/2}\pi^{-n/2}\left(\frac{\lambda}{\hbar}\right)^{n/2}\\ &\times\int_{\mathbb{C}^n}h'(z)^\dagger h(z)K(z,z^\dagger)^{\lambda/\hbar+1)/2}\,d\,\mathrm{Leb}^{2n},\end{aligned}$$

and for any observable f: $M\to\mathbb{R}$ we have (Theorem 2.1)

$$\langle h',\mathfrak{f}h\rangle=\langle h',[(1+\tfrac{1}{4}\hbar\Delta_{\mathrm{dR}})f]h\rangle \quad [\text{in } L^2(M,P)!].$$

The only remaining problem now is the determination of the structure of the (nontrivial) bundle QB. According to the general theory the bundle QB is the tensor product of the prequantum bundle L and a line bundle ML associated to the bundle of metalinear P frames. It is not true that both bundles do always exist: ML exists iff the first Chern class $c_1(\omega)^{\mathbb{R}}$ of the symplectic manifold is even, and L exists iff the symplectic form $\omega/\hbar$ determines an integer cohomology class, and QB exists iff $[\omega/\hbar]$ and $\frac{1}{2}c_1(\omega)^{\mathbb{R}}\in\mathbb{Z}$. However, if we are only interested in the bundle QB and not in the two constituents separately, then one can reduce the condition on existence to

$$[\omega/\hbar]+\tfrac{1}{2}c_1(\omega)^{\mathbb{R}}\in\mathbb{Z}, \tag{6.7}$$

a result which can be obtained by using Mp^c structures.[19] What we will do is to construct explicitly the transition functions of the bundle QB and then finding those values of λ for which this system of transition functions is indeed well defined, which in turn are those values of λ for which (6.7) is satisfied. Since $\epsilon_n=\text{const}\,K(z,z^\dagger)d\,\mathrm{Leb}^{2n}$ (6.5) is invariant under the action of G it follows that

$$K(gz,(gz)^\dagger)=\left|\frac{\partial gz}{\partial z}\right|^{-2}K(z,z^\dagger), \tag{6.8}$$

$$\frac{\partial gz}{\partial z}=\det(\text{Jacobian } (z\to gz)).$$

Now suppose that the holomorphic functions $h_i^{(\prime)}$ on U_i $(i=1,2)$ are local representations of global sections $\psi^{(\prime)}$ of QB, then from Sec. I we know that the function $H_{h',h}$ (1.1) is a global function on M, hence $h_1^{(\prime)}(z)=\mathrm{tr}_{12}(z)\cdot h_2^{(\prime)}(gz)$ [where g is the diffeomorphism (6.1) between the two charts $U_1\to U_2$ and where $\mathrm{tr}_{12}(z)$ is the transition function between the two trivializations above U_1 and U_2] implies

$$\begin{aligned}&h_1'(z)^\dagger h_1(z)K(z,z^\dagger)^{(\lambda/\hbar-1)/2}\\ &\quad=|\mathrm{tr}_{12}(z)|^2h_2'(gz)^\dagger h_2(gz)K(z,z^\dagger)^{(\lambda/\hbar-1)/2}\\ &\quad=h_2'(gz)^\dagger h_2(gz)K(gz,(gz)^\dagger)^{(\lambda/\hbar-1)/2}\\ &\quad=h_2'(gz)^\dagger h_2(gz)\left|\frac{\partial gz}{\partial z}\right|^{(1-\lambda/\hbar)}K(z,z^\dagger)^{(\lambda/\hbar-1)/2}\\ &\Rightarrow|\mathrm{tr}_{12}(z)|^2=\left|\frac{\partial gz}{\partial z}\right|^{(1-\lambda/\hbar)}.\end{aligned}$$

Because of the identification of local sections ψ which are covariant constant along P with holomorphic functions h, the transition functions are holomorphic (QB is in cases under investigation a holomorphic bundle). Since $\partial gz/\partial z$ is holomorphic, too, we deduce that

$$\mathrm{tr}_{12}(z)=\left(\frac{\partial gz}{\partial z}\right)^{(1-\lambda/\hbar)/2}. \tag{6.9}$$

Remark 6.1: If one computes the transition functions of the bundles L and ML seperately, one finds that for ML it is $(\partial gz/\partial z)^{1/2}$ and for L $(\partial gz/\partial z)^{-\lambda/\hbar/2}$, which also shows that for QB $=L\otimes$ ML the transition function is $(\partial gz/\partial z)^{1/2}\times(\partial gz/\partial z)^{-\lambda/\hbar/2}=(\partial gz/\partial z)^{(1-\lambda/\hbar)/2}$.

Remark 6.2: In reality one has a degree of freedom, one can modify (6.9) by a phase factor $\exp(i\varphi)$ (which vanishes when taking the absolute values). This freedom determines a Cech 1-cocycle with values in U(1) (the phase factor depends on the intersection $U_1\cap U_2$) and hence an element of $H^1(M,\mathrm{U}(1))$, which classifies the space of the inequivalent (pre)quantizations. However, each irreducible Hermitian symmetric space of compact type is simply connected, hence $H^1(M,\mathrm{U}(1))=\{0\}$, so modulo a natural equivalence of bundles L and QB our choice in (6.9) is unique.

We now want to "compute" the values of λ for which the transition functions (6.9) are well defined (perhaps by using subcharts on which the function $\zeta\to\zeta^{(1-\lambda/\hbar)/2}$ is defined) and for which they satisfy (at the same time) the cocycle condition $\mathrm{tr}_{12}\mathrm{tr}_{23}=\mathrm{tr}_{13}$.

Proposition 6.3: If $w=g^{-1}(0)\in\mathbb{C}^n$ *exists then*

$$\frac{\partial gz}{\partial z}=\text{const}(g)K(z,w^\dagger)=\text{const}\,N(z,w^\dagger)^{-\nu(M)}.$$

The proof of this proposition can be found in Ref. 12, Theorem 2.1. It can be verified easily for the spaces of type I, II, and III by using relation (6.8) to calculate $\partial gz/\partial z$ expli-

citly ($\Rightarrow \partial gz/\partial z = [\det(g_{21}z + g_{22})]^{-\nu(M)}$, a formula that is valid for all $g \in G$).

Corollary 6.4: $\mathrm{tr}_{12}(z) = \text{const} \cdot N(z,w^\dagger)^{(\lambda/\hbar - 1)\cdot\nu(M)/2}$.

In Ref. 12 it is shown that for the manifolds of type I, II, and IV $N(z,w^\dagger)$ is an irreducible polynomial in the unknowns $(z,w^\dagger)$ and for type III $N(z,w^\dagger)$ is the square of an irreducible polynomial. This fact is the main ingredient of the proof of the following theorem, a proof which will be delegated to the Appendix.

Theorem 6.5: (a) The values of λ for which the transition functions (6.9) define a bundle are given below [$\nu(M)$ is defined by (6.4)]:

$$\begin{aligned} &\tfrac{1}{2}(\lambda/\hbar - 1)\nu(M) \in \mathbb{Z}, && \text{for types I, II, and IV,} \\ &(\lambda/\hbar - 1)\nu(M) \in \mathbb{Z}, && \text{for type III,} \end{aligned} \tag{6.10}$$

or equivalently,

name	allowed λ's ($k \in \mathbb{Z}$)	name	allowed λ's ($k \in \mathbb{Z}$)
$M^{\mathrm{I}}_{p,q}$	$\dfrac{p+q+2k}{p+q}\hbar$	M^{III}_{p}	$\dfrac{p-1+k}{p-1}\hbar$
M^{II}_{p}	$\dfrac{p+1+2k}{p+1}\hbar$	M^{IV}_{p}	$\dfrac{p+2k}{p}\hbar$.

(b) For $0 < \lambda < \hbar$ *and* λ allowed (i.e., $\lambda > 0$ and $k < 0$) $\dim \mathscr{H} = 0$, for $\lambda = \hbar$ (i.e, $k = 0$) $\dim \mathscr{H} = 1$ and for $k > 0$: $0 < \dim \mathscr{H} < \infty$.

When we compare our allowed values with the allowed values of Berezin, we see that we can get a complete agreement if we identify our "parameter" $\frac{1}{2}(\lambda/\hbar - 1)$ [which appears in the transition function (6.9) and in the description of the inner product (6.6)] with the parameter h^{-1} of Berezin,[12] which appears in exactly the same way in the inner product. However, Berezin's definition of allowed values does not involve any condition on the bundle existence, it involves a certain condition on the Bergman kernel on the local chart $\mathbb{C}^n$ (see below). Since the allowed values agree, we may deduce that on the local chart U_{id} the (generalized) Bergman kernel $K_\lambda(z,w^\dagger)$ that is associated to the orthogonal projection $\pi: L^2(M,P) \to \mathscr{H}$ is given by

$$K_\lambda(z,w^\dagger) = \tilde{n}_\lambda(M) K(z,w^\dagger)^{(1-\lambda/\hbar)/2}$$

[in fact it is the validity of this relation between the function $K(z,w^\dagger)$ (6.2), (6.3), and the Bergman kernel K_λ that is the condition of Berezin], i.e., for $k \in L^2(M,P)$,

$$\begin{aligned} (\pi k)(w) &= c(M)^{-1/2}(\pi\lambda\hbar)^{-n/2} \int_{\mathbb{C}^n} K_\lambda(w,z^\dagger) k(z,z^\dagger) \\ &\quad \times K(z,z^\dagger)^{(\lambda/\hbar - 1)/2} \epsilon_n \\ &= c(M)^{-1/2}(\pi\lambda\hbar)^{-n/2} \tilde{n}_\lambda(M) \int_{\mathbb{C}^n} k(z,z^\dagger) \\ &\quad \times \left[\frac{K(z,z^\dagger)}{K(w,z^\dagger)}\right]^{(\lambda/\hbar - 1)/2} \epsilon_n . \end{aligned}$$

The constant $\tilde{n}_\lambda(M)$ is determined by $\tilde{n}_\lambda(M) = \|1\|^{-2}$, where $\|1\|$ is the norm of the global section ψ which is represented by the constant (holomorphic) function 1 on the local chart U_{id}; the branch of the function $\zeta \to \zeta^{(1-\lambda/\hbar)/2}$ is determined in the same way as for the tansition functions (6.9), $K_\lambda(z,w^\dagger)$ is a polynomial in $(z,w^\dagger)$ that is constant 1 for $z = 0$. As in Sec. V it follows that the set $\{e_w(z) = K_\lambda(z,w^\dagger) | w \in \mathbb{C}^n\}$ is a supercomplete system [with M° of Definition (3.1) given by the (local) chart $\mathbb{C}^n \cong U_{\mathrm{id}}$] and that for any observable $f: M \to \mathbf{R}$,

$$\mathrm{contravar}(\mathbf{f}) = (\mathbf{1} + \tfrac{1}{4}\hbar\Delta_{\mathrm{dR}})f.$$

As in the noncompact case we refer to Refs. 18 and 20 for the relation between covariant and contravariant symbols.

VII. SUMMARY AND DISCUSSION

In Sec. II we showed that on Kähler manifolds the geometric quantization scheme gives the following results: modulo a boundary term $\int d\alpha$ the operator $\mathbf{f}$ associated to a classical observable f is given by the process (1) multiply by $(\mathbf{1} + \frac{1}{4}\hbar\Delta_{\mathrm{dR}})f$ and then (2) take the holomorphic part ($\mathscr{H}$ is the subspace of holomorphic sections of QB with regard to the space of all "square integrable" sections of QB). For compact Kähler manifolds the boundary term $\int d\alpha$ is 0 and the above described result is exact. It was made plausible that for the physically interesting observables the result is also true on irreducible Hermitian symmetric spaces of noncompact type, from which one can deduce that it is true for all simply connected Hermitian symmetric spaces (see Ref. 10 Chap. VIII, §6). On the other hand, the above description of $\mathbf{f}$ can NOT be true in general: for $M = \{|z| < 1\} \subset \mathbb{C}$, $\omega = \frac{1}{2}i dz \wedge dz^\dagger$ and $f = z + z^\dagger$ (a *bounded* observable) the contribution $\int d\alpha$ is NOT zero for all $h, h' \in \mathscr{H}$.

In Secs. IV–VI we showed (forgetting for the moment about the boundary term) that on the *quantizable* irreducible Hermitian symmetric spaces (which gave a condition in the compact case) a supercomplete system (in the sense of Berezin) exists and that the contravariant symbol of any operator $\mathbf{f}$ associated to a classical observable f is given by $\mathrm{contrav}(\mathbf{f}) = (\mathbf{1} + \frac{1}{4}\hbar\Delta_{\mathrm{dR}})f$. Moreover, the quantization condition in the compact case coincides exactly with Berezin's definition of allowed values.

In order to relate our results to results obtained by *-product quantization we need a few comments on the close relationship between Berezin's quantization method and quantization by *-products. Both methods have as their basic assumption that quantum mechanics is a deformation of classical mechanics; the algebra of operators (especially observables) on the quantum mechanical Hilbert space depends upon a parameter $\hbar$ and in the limit $\hbar \downarrow 0$ this algebra reduces to the Poisson algebra of functions on the classical phase space (in quantum mechanics products of operators and commutators; in classical mechanics pointwise products of functions and Poisson brackets). More abstractly they study deformations (depending on a parameter) of the Poisson algebra. On the one hand Berezin realizes such a deformation as the set of *covariant* symbols of operators on a Hilbert space, deducing the product structure on these symbols from the product structure of the corresponding operators. On the other hand, *-products study such deformations abstractly. To compute physical relevant data (i.e., spectra of observables) they use a beautiful theorem[21] stating that to compute the spectrum of an "operator" [i.e., an element of the (deformed) algebra] one only needs the algebra structure, i.e., the *-product structure.

In Ref. 12 Berezin has computed the quantization on irreducible Hermitian symmetric spaces; for these cases the connection between covariant symbols and contravariant symbols and the associated *-products are calculated by Moreno in Refs. 16–18, 20. This gives us a way to compare the geometric quantization scheme with the quantization by *-products (deformations of the Poisson algebra), although the comparison works only in the case of Kähler manifolds (more precisely, for Hermitian symmetric spaces).

The results which have been discussed up till now are obtained by (conventional) geometric quantization including the metalinear correction. I now propose to "change" this quantization scheme in the case of positive Kähler polarizations: "hypothesis": the contravariant symbol of the operator $\mathbf{f}$ associated to the classical observable f is given by

$$f_{\text{contravar}} = \exp(\tfrac{1}{4}\hbar\Delta_{\text{dR}})f,$$

instead of $(1 + \frac{1}{4}\hbar\Delta_{\text{dR}})f$. At first this might seem a fancy change, but let us discuss the merits of this hypothesis. One of the first merits is that when we compare this quantization scheme in $\mathbb{C}^n$ [resulting in operators on the Bargmann representation) with the usual geometric quantization scheme on $\mathbb{C}^n$ with the vertical polarization [resulting in operators on the Schrödinger representation $\mathscr{H}_{\text{S}} = L^2(\mathbb{R}^n)$] then the results are the same for operators of the form $p^2 + pa(q) + V(q)$ (i.e., at most quadratic in the momentum variables). If $f_{\text{contravar}}$ had been given by $(1 + \frac{1}{4}\hbar\Delta_{\text{dR}})f$ then the results would have been different (see Ref. 1 for explicit calculations).

A second merit of our hypothesis can be found in the comparison with the Weyl–Wigner quantization scheme on $\mathbb{C}^n$. In Ref. 6 it is shown that the Weyl symbol f_{W} of an operator $\mathbf{f}$ is related to the contravariant symbol $f_{\text{contravar}}$ of the same operator by

$$f_{\text{W}} = \exp(-\tfrac{1}{4}\hbar\Delta_{\text{dR}})f_{\text{contravar}}.$$

With our hypothesis we find that $f_{\text{W}} = f$, i.e., the Weyl symbol is the classical observable we started with. It follows from the above observation that our hypothesis gives the same quantization prescription as the Weyl–Wigner quantization scheme, from which one deduces that our hypothesis gives on $\mathbb{C}^n$ the same quantization results as Berezin's and as the *-product approach (since these also coincide with the Weyl–Wigner procedure).

Apart from the above-mentioned merits of our hypothesis (i.e., giving the same results as various other quantization schemes) there is another merit: in Ref. 9 a problem was encountered in the (geometric) quantization of the classical hydrogen atom including spin: the hyperfine interaction term contains an incorrect factor $\frac{2}{5}$ (for $\frac{1}{2}$-densities the incorrect factor is $\frac{2}{3}$) that cannot be absorbed by rescaling. Assuming our hypothesis, this factor disappears (after reinterpreting the classical intrinsic angular momentum). More generally the situation is as follows: suppose we have two (isolated) physical systems without interaction, described by the symplectic (Kähler) manifolds (M_1,ω_1) and (M_2,ω_2). Then $(M_1\times M_2, \omega_1 + \omega_2)$ describes the two systems simultaneously and one can quantize it. Now suppose we consider observables f_1 on M_1 and f_2 on M_2, then $f(m_1,m_2) = f_1(m_1)f_2(m_2)$ is an observable on $M_1\times M_2$. Quantization of (M_i,ω_i) yields a Hilbert space $\mathscr{H}_i$ (of holomorphic sections of QB_i) and operators $\mathbf{f}_i$ on $\mathscr{H}_i$; quantization of $M_1\times M_2$ yields a Hilbert space $\mathscr{H}$ (which is in a certain sense the tensor product $\mathscr{H}_1 \otimes \mathscr{H}_2$) and one gets an operator $\mathbf{f}$ associated to $f = f_1 f_2$. When we now assume that after quantization the two systems should remain isolated (a reasonable assumption in physics), then one expects that

$$\left.\begin{aligned}&[\mathbf{f}_1,\mathbf{f}_2] = 0\\ &\mathbf{f} = \mathbf{f}_1\mathbf{f}_2.\end{aligned}\right\} \quad \text{(noninterference axiom)}.$$

Although the relation $[\mathbf{f}_1,\mathbf{f}_2] = 0$ is satisfied, the second relation $\mathbf{f} = \mathbf{f}_1\mathbf{f}_2$ is not satisfied. Investigating their contravariant symbols we find

$$\begin{aligned}&\text{contravar}(\mathbf{f})\\ &\quad = f_1 f_2 + \tfrac{1}{4}\hbar(\Delta_1 + \Delta_2)f_1 f_2\\ &\quad = f_1 f_2 + \tfrac{1}{4}\hbar f_1\Delta_2 f_2 + \tfrac{1}{4}\hbar f_2\Delta_1 f_1,\\ &\text{contravar}(\mathbf{f}_1\mathbf{f}_2)\\ &\quad = (f_1 + \tfrac{1}{4}\hbar\Delta_1 f_1)(f_2 + \tfrac{1}{4}\hbar\Delta_2 f_2)\\ &\quad = \text{contravar}(\mathbf{f}) + 16^{-1}\hbar^2(\Delta_1 f_1)(\Delta_2 f_2),\end{aligned}$$

so geometric quantization does not comply with our noninterference axiom [it is precisely the absence of the term $16^{-1}\hbar^2(\Delta_1 f_1)(\Delta_2 f_2)$ that explains the incorrect factor $\frac{2}{5}$ in the quantization of the hydrogen atom in Ref. 9]. On the other hand, our hypothesis, which changes the quantization results, does comply with the noninterference axiom:

$$\exp(\tfrac{1}{4}\hbar(\Delta_1 + \Delta_2))f_1 f_2 = [\exp(\tfrac{1}{4}\hbar\Delta_1)f_1][\exp(\tfrac{1}{4}\hbar\Delta_2)f_2].$$

At this point we must remember that our hypothesis is valid in the context of Kähler manifolds with their associated Kähler polarizations [so that $\mathscr{H}_i$ consists (locally) of holomorphic functions on M_i]. If M_1 and M_2 are two cotangent bundles $M_i = T^*Q_i$ and if we use the vertical polarizations ($\Rightarrow \mathscr{H}_i \cong$ functions on Q_i) then the axiom of noninterference is satisfied by the geometric quantization procedure (at least for the directly quantizable observables, i.e., the ones which are linear in p).

To summarize, the merits of our hypothesis are threefold: (1) the quantization results in $\mathbb{C}^n$ are the same as for Weyl–Wigner, Berezin, and *-products, (2) the quantization results in $\mathbb{C}^n$ are the same as for the vertical polarization, and (3) the quantization result satisfies the noninterference axiom.

Considering the above-mentioned arguments in favor of the hypothesis, I propose to change the geometric quantization scheme in such a way that the factor $(1 + \frac{1}{4}\hbar\Delta_{\text{dR}})$ in (2.3) is replaced by $\exp(\frac{1}{4}\hbar\Delta_{\text{dR}})$, i.e., considering geometric quantization as a first order approximation in $\hbar$ to "real" quantum mechanics. Unfortunately however, I have no conceptual idea how to change geometric quantization in order to obtain this result.

Remark 7.1: The arguments in favor of our hypothesis are arguments with physics in mind; from the point of view of representation theory of Lie groups this hypothesis is not so good. It should also be mentioned that the change $(1 + \frac{1}{4}\hbar\Delta_{\text{dR}}) \to \exp(\frac{1}{4}\hbar\Delta_{\text{dR}})$ does not explain the substitution $4\lambda^3 - 3\lambda^4 \to \lambda^2 J_0(-2i\log\lambda)$ made by Rawnsley and Sternberg in Ref. 22 to obtain (by means of geometric quantization) representations of $\text{SL}(3,\mathbb{R})$.

Remark 7.2: All preceding results concerning geometric quantization were derived by using the metalinear correction. When one uses $\frac{1}{2}$-densities instead of $\frac{1}{2}$-forms, there are some (minor) differences, some of which will be listed below.

(1) $H_{h'h}(z,z^\dagger) = (\pi\hbar)^{-n/2}h'(z)^\dagger h(z)\exp(-\frac{1}{2}f/\hbar)$ [formula (2.2)].

(2) $L_f h = -i\hbar X_f h + h\cdot\left[f - \dfrac{\partial F}{\partial z^j}\cdot g^{jk}\cdot\dfrac{\partial f}{\partial z^{k^\dagger}}\right]$.

(3) Starting at formula (2.3) the term $(1+\frac{1}{4}\hbar\Delta_{\mathrm{dR}})$ should be replaced everywhere by $(1+\frac{1}{4}\hbar\Delta_{\mathrm{dR}})$,

(4) The formulas $R_f(h'h) = d\alpha$, $\alpha = (-1)^{n-1}\times i\hbar H_{h'h}d''(f\epsilon_{n-1})$ remain valid (with the changed function $H_{h'h}$!).

(5) In Sec. V the exponent $-\frac{1}{2}(1+\lambda/\hbar)$ should be replaced by $-\frac{1}{2}\lambda/\hbar$ and in Sec. VI the exponent $\frac{1}{2}(\lambda/\hbar - 1)$ should be replaced by $\frac{1}{2}\lambda/\hbar$ (undoing of the metalinear correction).

The results with $\frac{1}{2}$-densities are exactly equal to results obtained by using prequantization only and restricting oneself to holomorphic sections.

APPENDIX: PROOF OF THEOREM 6.5

We start with some notations: (1) $\mu(g,z) = \partial gz/\partial z$ and (2) $\mathbb{C}(z)$ denotes the field of quotients of polynomials in the variables $z_1,\ldots,z^n$.

Proof of (a): sufficiency: We suppose that λ satisfies (6.10) and we have to prove that the transition functions (6.9) really define a holomorphic line bundle. Berezin proved in Ref. 12 that $N(z,w^\dagger)$ is (the square of) an irreducible polynomial in the unknowns $(z,w^\dagger)$, so it follows from Proposition 6.3, Corollary 6.4, and the condition (6.10) on λ that for certain $g\in G$ [i.e., $g^{-1}(0)$ should exist] that

$$\mathrm{tr}_{12}(z) = \mathrm{const}\circ N(z,w^\dagger)^{(\lambda/\hbar-1)\cdot\nu(M)/2}\in\mathbb{C}(z).$$

Since there exists a neighborhood of $\mathrm{id}\in G$ for which this condition on g is satisfied and since $\mu(g,z)$ (see above) satisfies the relation

$$\mu(g\cdot g',z) = \mu(g,g'z)\cdot\mu(g',z),$$

it follows that $\mathrm{tr}_{12}(z)\in\mathbb{C}(z)$ for all $g\in G$ [use that for nonzero constants there always exists a $[(\lambda/\hbar-1)\cdot\nu(M)/2]$ power and use that the components of gz are in $\mathbb{C}(z)$]. Hence for each pair of charts U_1 and U_2 connected by the element $g\in G$ the function $\mathrm{tr}_{12}(z)$ exists as a holomorphic function (in particular, as a quotient of polynomials).

The next step is to choose the functions $\mathrm{tr}_{12}(z)$ in such a way that they satisfy the cocycle condition, using the cover $\{U_g\,|\,g\in G\}$ (the different choices are different branches of the complex logarithm). For two charts U_g and $U_{g'}$ the connecting group element is $g'g^{-1}$ [see (6.1)] so $\mathrm{tr}_{(g,g')}(z)$ should be a choice for $\mu(g'g^{-1},z)^{(1-\lambda/\hbar)/2}$. We are going to define $\mathrm{tr}_{(g,g')}$ in two steps. We start with

$$\mathrm{tr}_{(e,g)}(z) = \mu(g,z)^{(1-\lambda/\hbar)/2}$$

with an arbitrary choice of the branch of the log [except for $\mathrm{tr}_{(e,e)}(z) = 1$)]. We know that $\mathrm{tr}_{(e,g)}(z)\in\mathbb{C}(z)$. Then we define

$$\mathrm{tr}_{(g,g')}(z) = \mathrm{tr}_{(e,g')}(g^{-1}z)/\mathrm{tr}_{(e,g)}(g^{-1}z)\in\mathbb{C}(z).$$

This $\mathrm{tr}_{(g,g')}(z)$ is for each fixed $z\in\mathbb{C}$ a $[(1-\lambda/\hbar)/2]$ power of $\partial(g'g^{-1})z/\partial z$, hence it is a holomorphic solution of (6.9) and moreover the system of transition functions $\mathrm{tr}_{(g,g')}(z)$ defined in this way obviously satisfies the cocycle relation

$$\mathrm{tr}_{(g,g')}(z)\cdot\mathrm{tr}_{(g',g'')}((g'g^{-1})z) = \mathrm{tr}_{(g,g'')}(z),$$

which proves that for λ's satisfying (6.10) there exists a line bundle QB with transition functions defined by (6.9). N.B. In general, one cannot expect that for any choice of branches $\mu(g,z)^{(1-\lambda/\hbar)/2}$ the relation $\mu(gh,z)^{(1-\lambda/\hbar)/2} = \mu(g,hz)^{(1-\lambda/\hbar)/2}\cdot\mu(h,z)^{(1-\lambda/\hbar)/2}$ is satisfied for all $g,h\in G$ simultaneously (there exist easy counterexamples); this fact shows the necessity of our detour by $\mathrm{tr}_{(e,g')}(z)$.

Proof of (a): necessity: We have seen that there exist λ's for which the line bundle QB is defined and in the same way one can show that there exist λ's for which the prequantum bundle L is defined. This shows that the group of periods of the symplectic form ω on M is discrete (see Ref. 15) and since M is compact it must be isomorphic to $\mathbb{Z}$, implying that the set of allowed values of λ is discrete (countably infinite). Hence there exists a smallest positive λ_0 for which L exists, and this λ_0 with the corresponding L_0 we will call the elementary prequantization. The general theory now shows that, given one quantum bundle $\mathrm{QB}(\lambda)$ for a certain value of λ, all other QB's (for other values of λ) can be obtained by tensoring with the elementary prequantization: $\mathrm{QB}(\lambda)\otimes L_0(\lambda_0) = \mathrm{QB}(\lambda+\lambda_0)$.

We know two obvious solutions λ_1 and λ_2: $\lambda_1 = \hbar$ [where QB is trivial: $\mathrm{tr}(z) = 1$, see (6.9)] and λ_2 defined by $(\lambda_2/\hbar - 1)\cdot\nu(M)/2 = 1$ (for type I, II, and IV; $\frac{1}{2}$ for type III) with $\mathrm{tr}(z) = \mathrm{const}\, S(z,w^\dagger)$, where $S(z,w^\dagger)$ is the irreducible polynomial from Berezin [$S(z,w^\dagger) = N(z,w^\dagger)$ for type I, II, and IV and $S(z,w^\dagger)^2 = N(z,w^\dagger)$ for type III]. From this we deduce that the difference $\lambda_2 - \lambda_1$ is an integer multiple k of λ_0.

Now choose any $g\in G$ such that $S(z,w^\dagger)$ has a simple zero in z [$w^\dagger$ depends on g; such a g exists, although it is not true, in general, that for all w $S(z,w^\dagger)$ should have a simple zero in z]. From $\lambda_2 - \lambda_1 = k\lambda_0$ it follows that $\mathrm{QB}(\lambda_2) \cong \mathrm{QB}(\lambda_1)\otimes\otimes^k L_0 \cong \otimes^k L_0$ [remember that $\mathrm{QB}(\lambda_1)$ is trivial]. Denote by $T(z)$ the transition function of L_0 between the two local charts U_e and U_g (our special g of above!) then by the bundle equivalence there exist nonzero holomorphic functions κ_e on U_e and κ_g on U_g such that $T = \kappa_e^{-1}S\kappa_g$. Since $U_e\cong U_g\cong\mathbb{C}^n$ there exist global k th roots of κ so there exists on $U_e\cap U_g$ a k th root of $S(z,w^\dagger)$. Because $U_e\cap U_g = \{z\in U_e\,|\,S(z,w^\dagger)\neq 0\}$ and because $S(z,w^\dagger)$ has a simple zero in z this leads to a contradiction except if $k = 1$, proving the necessity of condition (6.10).

Proof of (b): If $k = 0$ (i.e., $\lambda = \lambda_1$ and QB is trivial) then $\mathscr{H}$ consists of global holomorphic sections of the trivial bundle over a compact complex manifold, hence these sections must be constant, implying $\mathscr{H}\cong\mathbb{C}$. Another way to derive this result is by using the transition functions, if the global section ψ is represented on two local charts by $h_1(z)$ and $h_2(z)$ then $h_1(z) = h_2(gz)$. Now both $h_1(z)$ and $h_2(z)$ are

global holomorphic functions on $\mathbb{C}^n$ and gz is a quotient of polynomials with nonconstant denominator (in general) so $h_1(z)$ and $h_2(z)$ must be constant.

Now suppose $k<0$ (and $\lambda>0$) then we know from the proof of part (a) that $\mathrm{tr}_{12}(z) = \text{polynomial}(z)^k$ so the relation $h_1(z) = \mathrm{tr}_{12}(z)h_2(z)$ combined with $h_1(z)$ globally holomorphic shows that this is possible only if $h_1(z) = 0 = h_2(z)$, hence $\mathscr{H} = \{0\}$.

For $k>0$ the relation $h_1(z) = \mathrm{tr}_{12}(z)h_2(z)$ poses a condition on $h_1(z)$ and $h_2(z)$ which restricts these holomorphic functions to polynomials of fixed degree, so $\mathscr{H}$ is finite dimensional. The same conclusion can be obtained by inspecting the condition on the sections imposed by $\mathscr{H}$ [see (6.6)], h: $\mathbb{C}^n \to \mathbb{C}$ holomorphic is an element of $\mathscr{H}$ iff

$$\int |h(z)|^2 N(z,z^\dagger)^{-(\lambda/\hbar+1)\cdot\nu(M)/2}\, d\,\mathrm{Leb}^{2n} < \infty,$$

which also shows that h is restricted to polynomials of fixed degree [$N(z,z^\dagger)$ is a polynomial]. Q.E.D.

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A class of integrable potentials

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A class of time independent two-dimensional integrable potentials, all possessing an invariant of the same general form, is constructed. One of these potentials is superintegrable, its invariants realize the symmetry algebra sO(3) for negative energies, e(2) for zero energy, and sO(2,1) for positive energies. A transformation of coupling constants reveals that in parabolic coordinates this potential is the harmonic oscillator acted on by constant forces. This and another potential in the class may be considered as successive extensions of the Kepler potential. The analytic properties of these integrable systems in the complex time plane are also discussed.

I. INTRODUCTION

The study of integrable systems has witnessed a rapid growth in the past few years. Mostly study has focused on infinite-dimensional systems governed by nonlinear evolution equations. Of late, the identification and study of finite-dimensional integrable Hamiltonian systems has also proved to be of considerable interest. This has followed the realization that an arbitrary Hamiltonian system is likely to be nonintegrable and perhaps chaotic, the canonical example of such a system being the Hénon–Heiles system.[1] Interest in integrable Hamiltonian systems has been partly motivated by the practical need of realizing them in plasma physics and accelerators and partly by the desire to understand what characterizes integrability.

We will consider only two-dimensional, time-independent, classical Hamiltonian systems here. Such a system is integrable if there exists an additional analytic, single-valued, globally defined constant of the motion besides the energy. Darboux[2] may have been the first to give a systematic method of constructing a constant (or invariant) for a Hamiltonian system. In this direct method one postulates the form of the invariant, usually polynomial in the momenta. Demanding that the Poisson bracket of the invariant and the Hamiltonian vanish leads to a set of equations whose solution gives both the integrable potential and the complete invariant. This method has been used by several authors[3] to construct a variety of integrable potentials. Most of the results obtained up to now have been reviewed by Hietarinta.[4] All integrable potentials admitting invariants which are linear or quadratic in the momenta are known. At higher orders our knowledge is much less complete. The majority of results at higher order have been found by restricting the form of the invariant or making a particular choice for the form of the potential. In this paper we continue that tradition and choose our polynomial invariant to be of a certain allowable form and construct a class of integrable potentials which admit this type of invariant. There do exist other methods of identifying integrable systems, in particular, the Lax pair method,[5] and Painlevé analysis.[6] Indeed the latter has proved to be a useful complement to the direct method in integrability studies.

This paper is organized as follows. In Sec. II we introduce the method due to Darboux and write the particular choice of invariant. Assuming that the invariant is of nth order in the momenta, we find the necessary general form of a potential for it to admit an invariant of this type. In Sec. III and IV we carry out an explicit construction of the integrable potentials at $n = 3$ and $n = 4$, respectively. The potential we find in Sec. III,

$$V = \alpha z^{-1/2} + \beta \bar{z}^{-1/2} + \gamma (z\bar{z})^{-1/2}, \tag{1.1}$$

is superintegrable and turns out to be closely related to the two-dimensional Kepler potential. One of the four potentials we construct in Sec. IV can be viewed as the next extension of (1.1). In Sec. III we also look briefly at the quantum mechanics of (1.1) and obtain its energy spectrum by the use of its dynamical symmetry group. In Sec. V we perform a Painlevé analysis on the equations of motion of the integrable systems to test the nature of the singularities. Finally we conclude in Sec. VI with some remarks.

II. AN ANSATZ FOR THE INVARIANT

Consider the Hamiltonian to be of the standard form

$$H = \tfrac{1}{2}(p_x^2 + p_y^2) + V(x,y) \tag{2.1}$$

admitting a polynomial invariant (of nth order in the momenta) of the general form

$$I = \sum_{\substack{i=0 \\ i+j\le n}}^{n} \sum_{j=0}^{n} a_{ij}(x,y)\, p_x^i\, p_y^j\,, \tag{2.2}$$

where $i+j$ is either even or odd, according as n is even or odd.[7] The coefficients $a_{ij}(x,y)$ with total order $i+j=n$ can be determined to be[8]

$$a_{p\,n-p} = \sum_{r=0}^{n-p} \sum_{s=0}^{p} (-1)^s \binom{r+s}{r} A^{\,r+s}_{p-s\,n-p+s} x^r y^s, \qquad p = 0,1,\ldots,n, \tag{2.3}$$

where the $A^{\,k}_{ij}$ are constants whose values depend on the potential. So far most of the invariants known[4] with $n > 2$ are those where $a_{p\,n-p}$ are constants for all p. Thompson[9] and more recently Leach[10] and Sen[11] have considered invariants

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with

$$a_{p\,n-p} = (-1)^p \binom{n}{n-p} x^{n-p} y^p, \tag{2.4}$$

the invariant being

$$I = (xp_y - yp_x)^n + \text{lower-order terms.} \tag{2.5}$$

Here we concentrate on finding those integrable potentials for which

$$a_{p\,n-p} = (-1)^p \left[\binom{n-2}{n-p} x^{n-p} y^{p-2} + \binom{n-2}{n-p-2} x^{n-p-2} y^p \right], \tag{2.6}$$

i.e., the invariant is of the form

$$I = (xp_y - yp_x)^{n-2} (p_x^2 + p_y^2) + \text{lower-order terms.} \tag{2.7}$$

For I to be an invariant, its time derivative or equivalently its Poisson bracket with H (since I is explicitly time independent) must vanish. This condition results in a system of equations, the complete solution of which proceeds in two steps. First, we find that the potential V must obey an nth-order linear partial differential equation (PDE). The solution of this PDE determines V as a sum of n arbitrary functions of known arguments. Next, these arbitrary functions are subject to certain nonlinear equations. Solving these nonlinear equations in the second stage of the analysis is considerably simpler if we choose an appropriate coordinate system. This choice of coordinate system is indicated by the arguments of the functions appearing in the first step. For our choice of invariant (2.7), these natural coordinates are the complex coordinates. Complex coordinates were also used by Kaushal *et al.*[12] but no new integrable systems were found.

We now make the point transformation to complex coordinates and perform the analysis from the beginning in this system. The Hamiltonian (2.1) is now of the form

$$H = 2p_z p_{\bar z} + V(z,\bar z) \tag{2.8}$$

and the invariant (2.7) is

$$I(z,\bar z,p_z,p_{\bar z}) = (zp_z - \bar z p_{\bar z})^{n-2} p_z p_{\bar z} + \sum_{\substack{i=0 \\ i+j<n-2}}^{n-2} \sum_{j=0}^{n-2} c_{ij}(z,\bar z) p_z^i p_{\bar z}^j. \tag{2.9}$$

Here the coefficients $c_{ij}(z,\bar z)$ of total order $i+j=n$ are $(p = 1,...,n-1)$,

$$c_{p\,n-p} = (-1)^{n-p-1} \binom{n-2}{n-p-1} z^{p-1} \bar z^{n-p-1} \tag{2.10}$$

and

$$c_{n0} = 0 = c_{0n}. \tag{2.11}$$

The condition that the Poisson bracket of I and H vanish results in a system of equations $(i,j = 0,1,...,n-1)$,

$$2(\partial_z c_{ij-1} + \partial_{\bar z} c_{i-1\,j}) = (i+1) c_{i+1\,j}\, \partial_z V + (j+1) c_{ij+1}\, \partial_{\bar z} V, \tag{2.12}$$

obtained by equating the different powers of $p_z p_{\bar z}$ to 0. One must recall here the stipulation $c_{ij} = 0$ if $i,j<0$ or $i+j>n$.

The solution to this set of equations at a particular n determines the integrable potentials and the complete invariants.

Consider the following set of n equations $(j = 0,1...n-1)$:

$$2(\partial_z c_{n-j-1\,j-1} + \partial_{\bar z} c_{n-j-2\,j}) = (n-j) c_{n-j\,j}\, \partial_z V + (j+1) c_{n-j-1\,j+1}\, \partial_{\bar z} V \tag{2.13}$$

obtained from (2.12) by setting $i+j = n-1$. The nth-order linear PDE for V is obtained by eliminating the coefficients of order $(n-2)$ on the left-hand side from this system of equations. Some of these PDE's and their solutions (obtained by the method of characteristics) are

$$n = 3 \quad (z\,\partial_z^2\,\partial_{\bar z} - \bar z\,\partial_z\,\partial_{\bar z}^2) V = 0$$
$$\Rightarrow V(z,\bar z) = A(z) + B(\bar z) + C(z\bar z), \tag{2.14}$$

$$n = 4 \quad [z^2\partial_z^3\partial_{\bar z} - \bar z^2 \partial_z \partial_{\bar z}^3 + 5(z\partial_z^2\partial_{\bar z} - \bar z \partial_z \partial_{\bar z}^2)] V = 0$$
$$\Rightarrow V = A(z) + B(\bar z) + C(z\bar z) + (1/z\bar z) D(\bar z/z), \tag{2.15}$$

$$n = 5 [(z^3\partial_z^4\partial_{\bar z} + z^2\bar z \partial_z^3 \partial_{\bar z}^2 - z\bar z^2 \partial_z^2 \partial_{\bar z}^3 - \bar z^3 \partial_z \partial_{\bar z}^4) + 12(z^2\partial_z^3\partial_{\bar z} - \bar z^2 \partial_z \partial_{\bar z}^3) + 30(z\partial_z^2\partial_{\bar z} - \bar z \partial_z \partial_{\bar z}^2)] V = 0$$
$$\Rightarrow V = A(z) + B(\bar z) + C(z\bar z) + \frac{1}{z\bar z} D_1\left(\frac{\bar z}{z}\right) + \frac{1}{(z\bar z)^{3/2}} D_2\left(\frac{\bar z}{z}\right), \tag{2.16}$$

where $A,B,C,...$ are arbitrary functions of their arguments. It can be shown that at nth order the solution of the linear PDE is

$$V = A(z) + B(\bar z) + C(z\bar z) + \sum_{k=2}^{n-2} \frac{1}{(z\bar z)^{k/2}} D_k\left(\frac{\bar z}{z}\right). \tag{2.17}$$

This only completes the first stage of the analysis. At the second stage we find that these n arbitrary functions in (2.17) are also subject to $[n/2]-1$ additional nonlinear equations ($[n/2]$ is the smallest integer $\geqslant n/2$). The solutions to these nonlinear equations (which must be found at each value of n separately) determine the exact forms of the integrable potentials. In the following two sections we carry out this process at $n = 3,4$.

III. CUBIC INVARIANT

The invariant in complex coordinates is

$$I = (zp_z - \bar z p_{\bar z}) p_z p_{\bar z} + c_{10} p_z + c_{01} p_{\bar z}. \tag{3.1}$$

The equations determining c_{10} and c_{01} are [from (2.12)],

$$2\,\partial_{\bar z} c_{10} = z\,\partial_{\bar z} V,$$
$$2\,\partial_z c_{10} + 2\,\partial_{\bar z} c_{01} = 2(z\,\partial_z V - \bar z\,\partial_{\bar z} V), \tag{3.2}$$
$$2\,\partial_z c_{01} = -\bar z\,\partial_z V$$

and

$$c_{10}\,\partial_z V + c_{01}\,\partial_{\bar z} V = 0. \tag{3.3}$$

Eliminating c_{10} and c_{01} from (3.2) we get the PDE in (2.14). We now choose to write the solution as

$$V = A'(z) + B'(\bar z) + C(z\bar z). \tag{3.4}$$

The derivatives (denoted by primes) are taken for later convenience. The equations in (3.2) can now be solved for c_{10} and c_{01}. The general solution is

$$\begin{aligned} 2c_{10} &= 2zA'(z) - A(z) + zB'(\bar{z}) + zC(z\bar{z}), \\ 2c_{01} &= -[\bar{z}A'(z) + 2\bar{z}B'(\bar{z}) - B(\bar{z}) + \bar{z}C(z\bar{z})], \end{aligned} \tag{3.5}$$

where we have absorbed three arbitrary constants, one each in A,B, and C. The potential must also satisfy (3.3). This is a nonlinear compatibility condition that will determine the functional forms of A,B, and C. Substituting from (3.5), this equation can be written as

$$f(z) - g(\bar{z}) + h(z,\bar{z}) = 0, \tag{3.6}$$

where

$$\begin{aligned} f(z) &= (2zA' - A)A'', \quad g(\bar{z}) = (2\bar{z}B' - B)B'', \\ h(z,\bar{z}) &= [\bar{z}(zA' - A) - z(\bar{z}B' - B)]C' \\ &\quad + [zA'' - \bar{z}B'']C + zB'A'' - \bar{z}A'B''. \end{aligned} \tag{3.7}$$

To solve (3.6), set[13]

$$f(z) = a, \quad g(\bar{z}) = b, \quad h(z,\bar{z}) = b - a, \tag{3.8}$$

where a and b are constants. The first two equations in (3.8) are used to determine A and B, respectively, and then the last can be used to find C. The general solution of

$$f(z) = (2zA' - A)A'' = a,$$

where $a \neq 0$ can only be given in the parametric form

$$\begin{aligned} A(z) &= z(t - a/t) + k_1/t, \\ z &= t^2 \exp\left(\frac{t^2}{2a}\right)\left\{\frac{k_1}{a}\frac{d}{da^{-1}}\left[\sqrt{2a}\,\mathrm{erf}\left(\frac{t}{\sqrt{2a}}\right)\right] + k_2\right\}, \end{aligned} \tag{3.9}$$

where t is the parameter, k_1 and k_2 are arbitrary constants. A similar solution holds for $B(\bar{z})$ with $b \neq 0$. The last of (3.8) can be written in the form

$$\begin{aligned} &\partial_z[(zA' - A)(B' + C)] \\ &\quad - \partial_{\bar{z}}[(\bar{z}B' - B)(A' + C)] = b - a. \end{aligned} \tag{3.10}$$

This equation together with the above solutions for $A(z)$ and $B(\bar{z})$ has not proved tractable when either of a, b or both are nonzero, nor even in the case $b - a = 0$. The question whether there do exist solutions to (3.8) under the above conditions is left open. However, it can be shown that there is no solution with A, B, and C analytic in their arguments, which is compatible with (3.10) and the solution for $A(z)$ and $B(\bar{z})$ obtained above.

With $a = 0 = b$, $A(z)$ and $B(\bar{z})$ are given by

$$A(z) = \alpha z^{1/2}, \quad B(\bar{z}) = \beta\bar{z}^{1/2}, \tag{3.11}$$

where α, β are arbitrary constants, complex in general. [We can ignore the cases $A''(z) = 0 = B''(\bar{z})$ since they lead to a potential with spherical symmetry.] The equation for C now reduces to

$$2z\bar{z}C' + C = 0, \tag{3.12}$$

with the solution

$$C(z\bar{z}) = \gamma(z\bar{z})^{-1/2}, \tag{3.13}$$

where γ is an arbitrary constant, complex in general. The integrable Hamiltonian is

$$H = 2p_z p_{\bar{z}} + \alpha z^{-1/2} + \beta\bar{z}^{-1/2} + \gamma(z\bar{z})^{-1/2} \tag{3.14}$$

(after rescaling α,β) and is complex in general. As we will see, this system turns out to be closely related to the Kepler potential. Most real integrable systems remain integrable under complex extension but complex integrable potentials by themselves have also been considered before (see, e.g., Hietarinta[14]). Physically we will be interested only in the real versions but for the purpose of studying integrability we work with the general complex potential. To complete the determination of the invariant, the coefficients c_{10} and c_{01} may be found using (3.5). The complete invariant is

$$\begin{aligned} I = (zp_z - \bar{z}p_{\bar{z}})p_z p_{\bar{z}} &+ \tfrac{1}{2}[\beta\bar{z}^{-1/2} + \gamma(z\bar{z})^{-1/2}]zp_z \\ &- \tfrac{1}{2}[\alpha z^{-1/2} + \gamma(z\bar{z})^{-1/2}]\bar{z}p_{\bar{z}}. \end{aligned} \tag{3.15}$$

Before we discuss the system (3.14) in detail, let us consider the possibility of other solutions to (3.6), with $a = 0 = b$. If A and B both vanish then C can be arbitrary. The potential is spherically symmetric and the Hamiltonian admits a linear invariant, the angular momentum. In all other cases, e.g., if only one of A, B, C vanishes, then it is straightforward to show that the only possible solutions are special cases of (3.14).

The Hamiltonian (3.14) reduces to the two-dimensional Kepler system when $\alpha = 0 = \beta$. That system has the angular momentum and the two components of the Runge–Lenz vector as invariants. Checking for lower-order invariants we find that the above system also admits two quadratic invariants

$$\begin{aligned} I_1 &= (zp_z - \bar{z}p_{\bar{z}})p_z \\ &\quad + \tfrac{1}{2}[\beta\bar{z}^{1/2} - \alpha z^{-1/2}\bar{z} - \gamma z^{-1/2}\bar{z}^{1/2}], \end{aligned} \tag{3.16}$$

$$\begin{aligned} I_2 &= (zp_z - \bar{z}p_{\bar{z}})p_{\bar{z}} \\ &\quad + \tfrac{1}{2}[\beta z\bar{z}^{-1/2} - \alpha z^{1/2} - \gamma z^{1/2}\bar{z}^{-1/2}]. \end{aligned} \tag{3.17}$$

Thus this system has four invariants including the energy. For an autonomous system with s degrees of freedom there may exist only $2s - 1$ independent invariants for the system to be able to evolve in time. The invariants constructed here are related by the algebraic equation

$$(I_1 I_2 + \tfrac{1}{4}\gamma^2)H + \tfrac{1}{2}(\alpha^2 I_1 - \beta^2 I_2) + \tfrac{1}{2}\alpha\beta\gamma = 2I_3^2, \tag{3.18}$$

where the cubic invariant has been relabeled I_3. With $\alpha = 0 = \beta$, I_1 and I_2 reduce to the two components of the Runge–Lenz vector and I_3 to the product of the angular momentum and the energy. The existence of the quadratic invariants implies that the Hamilton–Jacobi equation separates in one of the orthogonal coordinate systems. The system above separates in parabolic coordinates ζ_1,ζ_2: $z = (\zeta_1 + i\zeta_2)^2$; in which the Hamiltonian is

$$\begin{aligned} H = \frac{1}{\zeta_1^2 + \zeta_2^2}\Bigg[\frac{1}{2}(p_{\zeta_1}^2 + p_{\zeta_2}^2) \\ + (\alpha + \beta)\zeta_1 + i(\beta - \alpha)\zeta_2 + \gamma\Bigg]. \end{aligned} \tag{3.19}$$

This is real valued if we take $\beta = \alpha^*$ and it turns out to be one of the four potentials found by Winternitz *et al.*[15] for which the Hamilton–Jacobi equation separates in two coordinate systems (here two parabolic coordinate systems mu-

tually perpendicular to each other) and thus admits two independent quadratic invariants. Consider the physically more interesting case of the real potential. Define the following real-valued invariants:

$$J_1 = i(\epsilon/2H)^{1/2}[I_1 + I_2 + (1/2H)(\alpha^2 - \alpha^{*2})],$$
$$J_2 = (\epsilon/2H)^{1/2}[I_1 - I_2 - (1/2H)(\alpha^2 + \alpha^{*2})], \qquad (3.20)$$
$$J_3 = -(2i/H)I_3,$$

where $\epsilon = \operatorname{sgn} H$. The Poisson bracket relations between them are

$$\{J_1,J_2\} = -\epsilon J_3, \quad \{J_2,J_3\} = J_1, \quad \{J_3,J_1\} = J_2. \qquad (3.21)$$

Thus the Poisson algebra is isomorphic to the Lie algebra of SO(3) for negative energies, to E(2) for zero energy, and to SO(2,1) for positive energies, respectively. This of course is also true for the two-dimensional Kepler potential. The realization of a dynamical symmetry group (energy dependent) by the invariants singles out this potential from the other three potentials found by Winternitz *et al.*[15] These potentials are

$$\text{(i) } V = \alpha(x^2 + y^2) + \beta_1 x^{-2} + \beta_2 y^{-2}$$
$$= \alpha r^2 + (1/r^2)[\beta_1 \sec^2\theta + \beta_2 \csc^2\theta],$$
$$\text{(ii) } V = \alpha(4x^2 + y^2) + \beta x + \gamma y^{-2}$$
$$= [1/(\zeta_1^2 + \zeta_2^2)][4\alpha(\zeta_1^6 + \zeta_2^6) + \beta(\zeta_1^4 - \zeta_2^4) + (\gamma/4)(\zeta_1^{-2} + \zeta_2^{-2})],$$
$$\text{(iii) } V = \frac{\alpha}{2r} + \frac{1}{4r^2}\left[\beta_1 \sec^2\frac{\theta}{2} + \beta_2 \csc^2\frac{\theta}{2}\right]$$
$$= \frac{1}{\zeta_1^2 + \zeta_2^2}[\alpha + \beta_1\zeta_1^{-2} + \beta_2\zeta_2^{-2}], \qquad (3.22)$$

where (r,θ) are the polar coordinates and (ζ_1,ζ_2) are parabolic coordinates. The configuration paths in each of the four potentials are closed periodic trajectories. Furthermore, potential (iii) also reduces to the Kepler potential when $\beta_1 = 0 = \beta_2$. However, for these three potentials, the invariants do not close under the Poisson bracket operation to give a finite-dimensional algebra. Classically at least, these potentials do not admit a symmetry group even though their motions are completely degenerate.

Besides the harmonic oscillator, the Kepler potential, and the four-potentials mentioned above, at least three other potentials are known to be superintegrable (i.e., admit three algebraically independent invariants) in two dimensions. In an arbitrary number of dimensions N the known superintegrable potentials, admitting $2N - 1$ independent invariants, are again the harmonic oscillator and the Kepler potential. It would be interesting to check if the higher-dimensional analogs of the potentials listed in (3.22) and in particular of (3.19), are superintegrable or not.

The close connection of the system (3.19) to the Kepler system can also be seen in the following way. It is well known that under the time coordinate transformation

$$t \to s; \frac{ds}{dt} = (\zeta_1^2 + \zeta_2^2)^{-1},$$

the Kepler potential is transformed into the harmonic oscillator when expressed in parabolic coordinates.[16] We have

$$\frac{d\zeta_1}{ds} = p_{\zeta_1}, \quad \frac{d\zeta_2}{ds} = p_{\zeta_2},$$

and the energy equation (3.19) for the real potential can be written as

$$-\gamma = (\tfrac{1}{2}p_{\zeta_1}^2 + \tfrac{1}{2}p_{\zeta_2}^2) - E(\zeta_1^2 + \zeta_2^2) + \kappa_1\zeta_1 + \kappa_2\zeta_2, \qquad (3.23)$$

where $\kappa_1 = \alpha + \alpha^*$, $\kappa_2 = i(\alpha^* - \alpha)$ are real constants. Here $-\gamma$ can be interpreted as the Hamiltonian for a two-dimensional isotropic harmonic oscillator (with coupling constant $-E$) acted on by a constant force. This noncanonical time transformation also serves as an example of a coupling constant metamorphosis between two integrable systems.[17]

One may try to look for a geometrical reason behind the degeneracy of the system (3.19), given that it is so closely related to the Kepler sytem. The Kepler potential is of course spherically symmetric but in addition, the equations of motion resulting from it are invariant under the transformation

$$\mathbf{r} \to \mathbf{r}(1 + \mathbf{c}\cdot\mathbf{r})^{-1}, \quad dt \to dt(1 + \mathbf{c}\cdot\mathbf{r})^{-2},$$

where $\mathbf{c}$ is an arbitrary constant vector. This invariance has been shown to lead to the conservation of the Runge–Lenz vector.[18] No such invariance transformation (i.e., a point transformation in space) exists here. Again, unlike the Kepler potential, the equations of motion of (3.19) do not admit any finite, nontrivial (i.e., besides time translation) space-time symmetry transformation. See the Appendix for the proof. Alternatively one might try transforming to momentum space, as was done for the hydrogen atom by Fock who reduced the motion by a stereographic projection to free flow on a hypersphere (for bound states) or on a hyperboloid (for scattering states). The reason why this works is that the invariants for the Kepler potential involve the space coordinates only linearly or have $1/r$ whose Fourier transform is simple. In our case, the nonlinear terms occurring with α, β in (3.15)–(3.17) would appear to rule out such a simple picture in momentum space. Thus the realization of the space on which the motion of the system (3.19) would be a free flow is still left open.

Let us look briefly at the quantum mechanics of this system. The presence of the quadratic invariants implies that the quantum version of this potential is integrable too.[19] The quantum invariants can be calculated from (3.15)–(3.17) by use of either of the symmetrization, Born–Jordan, or Wigner–Weyl correspondence rules[20] to get

$$\hat{I}_1 = (zp_z - \bar{z}p_{\bar{z}})p_z - (i/2)p_z + \tfrac{1}{2}(\beta\bar{z}^{1/2} - \alpha z^{-1/2}\bar{z} - \gamma z^{-1/2}\bar{z}^{1/2}),$$
$$\hat{I}_2 = (zp_z - \bar{z}p_{\bar{z}})p_{\bar{z}} + (i/2)p_{\bar{z}} + \tfrac{1}{2}(\beta z\bar{z}^{-1/2} - \alpha z^{1/2} + \gamma z^{1/2}\bar{z}^{-1/2}), \qquad (3.24)$$
$$\hat{I}_3 = (zp_z - \bar{z}p_{\bar{z}})p_z p_{\bar{z}} + \tfrac{1}{2}(\beta\bar{z}^{-1/2} + \gamma(z\bar{z})^{-1/2})zp_z - \tfrac{1}{2}(\alpha z^{-1/2} + \gamma(z\bar{z})^{-1/2})\bar{z}p_{\bar{z}} + (i/8)(\alpha z^{-1/2} - \beta\bar{z}^{-1/2}).$$

The relation (3.18) between the invariants is altered to

$$(\hat{I}_1\hat{I}_2 + i\hat{I}_3 + \tfrac{1}{4}\gamma^2)\hat{H} + \tfrac{1}{2}(\alpha^2\hat{I}_1 - \beta^2\hat{I}_2) + \tfrac{1}{2}\alpha\beta\gamma = 2(\hat{I}_3^2 - \tfrac{1}{16}\hat{H}^2). \tag{3.25}$$

For the real potential the same expressions as in (3.20) can be used to define the quantities $\hat{J}_1, \hat{J}_2, \hat{J}_3$. Now the commutator algebras of these invariants yields the same Lie algebras as in the classical case. Following Pauli's derivation of the hydrogen spectrum, the bound state energy spectrum of this model can be obtained by using the Casimir operator for SO(3),

$$C = \hat{J}_1^2 + \hat{J}_2^2 + \hat{J}_3^2 = -\left(\frac{1}{4} + \frac{1}{2\hat{H}}\left(\gamma^2 + \frac{2|\alpha|^2\gamma}{\hat{H}} + \frac{|\alpha|^4}{\hat{H}^2}\right)\right) \tag{3.26}$$

[using (3.25)]. Equating this to the eigenvalues of C, viz, $j(j+1)$ where $j = 0, \frac{1}{2}, 1, \ldots$ we get the energy eigenvalue equation ($n = 2j+1 = 1,2,3\ldots$),

$$n^2E^3 + 2\gamma^2E^2 + |\alpha|^2\gamma E + 2|\alpha|^4 = 0, \tag{3.27}$$

a result also obtained by Winternitz *et al.*[15] by solving the Schrödinger equation.

Analogous to the classical result, the commutator algebra of the quantum invariants for the potentials in (3.22) does not close. However, the symmetry group SU(2) [or O(3), locally isomorphic to it] can be realized at the quantum mechanical level by defining appropriate ladder operators.[15]

IV. QUARTIC INVARIANT

The invariant is

$$I = (zp_z - \bar{z}p_{\bar{z}})^2 p_z p_{\bar{z}} + c_{20}p_z^2 + c_{11}p_z p_{\bar{z}} + c_{02}p_{\bar{z}}^2 + c_{00}. \tag{4.1}$$

The system of equations (2.12) at $n = 4$ reduces to

$$\begin{aligned} 2\partial_{\bar{z}}c_{20} &= z^2\partial_{\bar{z}}V, \\ 2\partial_z c_{20} + 2\partial_{\bar{z}}c_{11} &= 3z^2\partial_z V - 4z\bar{z}\partial_{\bar{z}}V, \\ 2\partial_z c_{11} + 2\partial_{\bar{z}}c_{02} &= -4z\bar{z}\partial_z V + 3\bar{z}^2\partial_{\bar{z}}V, \\ 2\partial_z c_{02} &= \bar{z}^2\partial_z V \end{aligned} \tag{4.2}$$

and

$$\begin{aligned} 2\partial_z c_{00} &= c_{11}\partial_z V + 2c_{02}\partial_{\bar{z}}V, \\ 2\partial_{\bar{z}}c_{00} &= 2c_{20}\partial_z V + c_{11}\partial_{\bar{z}}V. \end{aligned} \tag{4.3}$$

Differentiating thrice to eliminate the coefficients on the left-hand side of (4.2) we find that the potential obeys the linear PDE (2.15). As before, we write the general solution for V as

$$V(z,\bar{z}) = A'(z) + B'(\bar{z}) + C(z\bar{z}) + (1/z\bar{z})D(\bar{z}/z). \tag{4.4}$$

The coefficients at order 2 may be obtained by integrating (4.2) to get the general solution

$$\begin{aligned} c_{20} &= \tfrac{1}{2}[3z^2A' - 2zA + z^2B' + z^2C + zD/\bar{z} + k_2], \\ c_{11} &= -[\bar{z}(2zA' - A) + z(2\bar{z}B' - B) + z\bar{z}C + 3D + k_1], \\ c_{02} &= \tfrac{1}{2}[\bar{z}^2A' + 3\bar{z}^2B' - 2\bar{z}B + \bar{z}^2C + (\bar{z}/z)D + k_0], \end{aligned} \tag{4.5}$$

where k_0, k_1, k_2 are arbitrary constants. Two other constants have been absorbed in A and B. The nonlinear compatibility condition on V can be obtained by eliminating c_{00} from (4.3). It is

$$[2c_{20}\partial_z^2 - 2c_{02}\partial_{\bar{z}}^2 + (2\partial_z c_{20} - \partial_{\bar{z}}c_{11})\partial_z + (\partial_z c_{11} - 2\partial_{\bar{z}}c_{02})\partial_{\bar{z}}]V = 0. \tag{4.6}$$

As was the case for the cubic invariant, this can be written in the form

$$f(z) - g(\bar{z}) + h(z,\bar{z}) = 0, \tag{4.7}$$

where

$$\begin{aligned} f(z) &= (3z^2A' - 2zA + k_2)A''' + 3(z^2A'' + 2zA' - A)A'', \quad g(\bar{z}) = (3\bar{z}^2B' - 2\bar{z}B + k_0)B''' + 3(\bar{z}^2B'' + 2\bar{z}B' - B)B'', \\ h(z,\bar{z}) &= [2\bar{z}^2(z^2A' - zA) - 2z^2(\bar{z}^2B' - \bar{z}B) + k_2\bar{z}^2 - k_0z^2]C'' + 3[\bar{z}(z^2A'' + zA' - A) - z(\bar{z}^2B'' + \bar{z}B' - B)]C' \\ &\quad + [z^2A''' + 3zA'' - \bar{z}^2B''' - 3\bar{z}B'']C + \frac{1}{z^4}\left[2\bar{z}(zA' - A) - 2z(\bar{z}B' - B) + k_2\frac{\bar{z}}{z} - k_0\frac{z}{\bar{z}}\right]D''' \\ &\quad + \frac{1}{z^2}\left[-\frac{1}{z}(3z^2A'' - 5zA' + 5A) - \frac{1}{\bar{z}}(3\bar{z}^2B'' - \bar{z}B' + B) + \frac{4k_2}{z^2} - \frac{2k_0}{\bar{z}^2}\right]D'' + \frac{1}{z\bar{z}}\left[\frac{1}{z}(z^3A''' + zA' - A)\right. \\ &\quad \left. - \frac{1}{\bar{z}}(\bar{z}^3B''' + \bar{z}B' - B) + \frac{k_2}{z^2} - \frac{k_0}{\bar{z}^2}\right]D + (z^2A''' + 3zA'')B' - A'(\bar{z}^2B''' + 3\bar{z}B''). \end{aligned} \tag{4.8}$$

On the grounds of tractability, we solve (4.7) by setting each of f, g, and h to 0 and look for power law solutions for $A(z)$ and $B(\bar{z})$. This also requires $k_2 = 0 = k_0$. The power law solutions obtained from $f(z) = 0$ are

$$A(z) = z, z^{1/2}, z^{1/3},$$

and similarly for $B(\bar{z})$. Writing $A(z) = \alpha z^r$, $B(\bar{z}) = \beta\bar{z}^s$, where α, β are arbitrary complex constants, the equation $h(z,\bar{z}) = 0$ reduces to

$$\begin{aligned} &[2\alpha(r-1)z^{r+1}z^s - 2\beta(s-1)z^2\bar{z}^{s+1}]C'' + 3[\alpha(r-1)(r+1)z^r\bar{z} - \beta(s-1)(s+1)z\bar{z}^s]C' + [\alpha r(r-1)(r+1)z^{r-1} \\ &\quad - \beta s(s-1)(s+1)\bar{z}^{s-1}]C + z^{-4}[2\alpha(r-1)z^r\bar{z} - 2\beta(s-1)z\bar{z}^s]D'' + z^{-2}[-\alpha(r-1)(3r-5)z^{r-1} \\ &\quad - \beta(s-1)(3s-1)\bar{z}^{s-1}]D' + z^{-1}\bar{z}^{-1}[\alpha(r-1)^3z^{r-1} - \beta(s-1)^3\bar{z}^{s-1}]D - \alpha\beta rs[(r-1)(r+1) \\ &\quad - (s-1)(s+1)]z^{r-1}\bar{z}^{s-1} = 0. \end{aligned} \tag{4.9}$$

This is a linear equation for the two functions $C(z\bar{z})$ and $D(\bar{z}/z)$. It will be solved by the method of separating variables. There are six distinct values for the pair (r,s): $(1,1)$, $(1,\frac{1}{2})$, $(1,\frac{1}{3})$, $(\frac{1}{2},\frac{1}{2})$, $(\frac{1}{2},\frac{1}{3})$, $(\frac{1}{3},\frac{1}{3})$. With $r=1, A'(z)$ reduces to a constant and can be dropped from the potential, i.e., we can put $\alpha=0$ for $r=1$. Similarly for $s=1$, set $\beta=0$.

Consider first $(r,s)=(1,1)$. In this case (4.9) is satisfied identically so C and D can be completely arbitrary. The Hamiltonian is

$$H=2p_zp_{\bar{z}}+C(z\bar{z})+(1/z\bar{z})D(\bar{z}/z)$$
$$\equiv\frac{1}{2}\left(p_r^2+\frac{1}{r^2}p_\theta^2\right)+F(r)+\frac{1}{r^2}G(\theta), \tag{4.10}$$

where r, θ are the polar coordinates. For this system the Hamilton–Jacobi equation separates in polar coordinates,[21] thus there exists an invariant quadratic in the momenta. The quartic invariant found here is just the product of that invariant and the Hamiltonian.

We give as an example, the method of solution for one of the other cases, $(r,s)=(\frac{1}{2},\frac{1}{2})$. On separating variables, (4.9) reduces to

$$8\xi^2C''+18\xi C'+3C=\lambda\xi^{-1},$$
$$8(\alpha\eta^{1/2}-\beta)\eta^2D''+2(7\alpha\eta^{1/2}-\beta)\eta D'$$
$$+(\alpha\eta^{1/2}-\beta)D=-\lambda(\alpha\eta^{1/2}-\beta),$$

where $\xi=z\bar{z}$, $\eta=\bar{z}/z$, $C=C(\xi)$, $D=D(\eta)$, and λ is the separation constant. These equations have the solutions

$$C=\mu_1\xi^{-1/2}+\mu_2\xi^{-3/4}+\lambda\xi^{-1},$$
$$D=(\eta^{1/2}-\delta)^{-2}[\nu_1\eta^{1/4}(\eta^{1/2}+\delta)+\nu_2\eta^{1/2}]-\lambda,$$

where $\delta=\beta/\alpha$ and μ_1,μ_2,ν_1,ν_2 are arbitrary complex constants. The potential is

$$V(z,\bar{z})=\alpha z^{-1/2}+\beta\bar{z}^{-1/2}+\mu_1\xi^{-1/2}+\mu_2\xi^{-3/4}$$
$$+\xi^{-1}(\eta^{1/2}-\delta)^{-2}[\nu_1\eta^{1/4}(\eta^{1/2}+\delta)+\nu_2\eta^{1/2}]. \tag{4.11}$$

The λ terms cancel out and we have rescaled α,β.

For the case $(\frac{1}{2},\frac{1}{3})$ it is easy to show that there exists no solution to (4.9). In the other three cases the analysis proceeds similarly.

Thus we have four new and distinct cases of integrable potentials with quartic invariants

$$\text{(I) } V(z,\bar{z})=\beta\bar{z}^{-1/2}+\mu_1\xi^{-1/2}+\mu_2\xi^{-3/4}+\xi^{-1}\times[\nu_1\eta^{1/4}+\nu_2\eta^{1/2}],$$
$$\text{(II) } V(z,\bar{z})=\beta\bar{z}^{-2/3}+\mu_1\xi^{-1/3}+\mu_2\xi^{-2/3}+\xi^{-1}\times(\nu_1\eta^{1/3}+\nu_2\eta^{2/3}),$$
$$\text{(III) } V(z,\bar{z})=\alpha z^{-1/2}+\beta\bar{z}^{-1/2}+\mu_1\xi^{-1/2}+\mu_2\xi^{-3/4}+\xi^{-1}(\eta^{1/2}-\delta)^{-2}\times[\nu_1\eta^{1/4}(\eta^{1/2}+\delta)+\nu_2\eta^{1/2}],$$

TABLE I. Integrable potentials with quartic invariants.

Potential	Invariant
$V=A'(z)+B'(\bar{z})+C(\xi)+\xi^{-1}D(\eta)$	$I=I_4+I_2$
	$I_4=(zp_z-\bar{z}p_{\bar{z}})^2p_zp_{\bar{z}}$
$\xi=z\bar{z},\quad \eta=\bar{z}/z$	I_2
(I) $\beta\bar{z}^{-1/2}+\mu_1\xi^{-1/2}+\mu_2\xi^{-3/4}+\xi^{-1}(\nu_1\eta^{1/4}+\nu_2\eta^{1/2})$	$\frac{1}{2}(B'+C+\xi^{-1}D)z^2p_z^2-(C+3\xi^{-1}D)\xi p_zp_{\bar{z}}+\frac{1}{2}(-B'+C+\xi^{-1}D)\bar{z}^2p_{\bar{z}}^2$ $-\{(\nu_1+\nu_2\eta^{1/4})[\mu_1z^{-3/4}\bar{z}^{-1/4}+\nu_2z^{-1}\bar{z}^{-1/2}+z^{-3/2}\bar{z}^{-1/2}(\nu_1+\nu_2\eta^{1/4})]$ $+(\beta/4)(\mu_2\eta^{-1/4}-\nu_1\xi^{-1/4}+\beta z)\}$
(II) $\beta\bar{z}^{-2/3}+\mu_1\xi^{-1/3}+\mu_2\xi^{-2/3}+\xi^{-1}(\nu_1\eta^{1/3}+\nu_2\eta^{2/3})$	$\frac{1}{2}(B'+C+\xi^{-1}D)z^2p_z^2+(B'-C-3\xi^{-1}D)\xi p_zp_{\bar{z}}+\frac{1}{2}(-3B'+C+\xi^{-1}D)\bar{z}^2p_{\bar{z}}^2$ $-\{(\nu_1+\nu_2\eta^{1/3})[\mu_1z^{-2/3}+\mu_2z^{-1}\bar{z}^{-1/3}+z^{-5/3}\bar{z}^{1/3}(\nu_1+\nu_2\eta^{1/3})]$ $+\beta z^{2/3}(\mu_2\xi^{-1/3}+\nu_2z^{-4/3}+\beta\eta^{-1/3})\}$
(III) $\alpha z^{-1/2}+\beta\bar{z}^{-1/2}+\mu_1\xi^{-1/2}+\mu_2\xi^{-3/4}+\xi^{-1}(\eta^{1/2}-\delta)^{-2}\times[\nu_1\eta^{1/4}(\eta^{1/2}+\delta)+\nu_2\eta^{1/2}]$	$\frac{1}{2}(-A'+B'+C+\xi^{-1}D)z^2p_z^2-(C+3\xi^{-1}D)\xi p_zp_{\bar{z}}+\frac{1}{2}(A'-B'+C+\xi^{-1}D)\bar{z}^2p_{\bar{z}}^2$ $+\frac{1}{2}\mu_2(\alpha\eta^{1/4}+\beta\eta^{-1/4})-\frac{1}{2}\nu_1\xi^{-1/4}+\frac{1}{4}(\alpha\bar{z}^{1/2}-\beta z^{1/2})^2-(\eta^{1/2}-\delta)^{-2}z^{-1}$ $\times[\nu_1(\mu_1\eta^{-1/4}+\mu_2\bar{z}^{-1/2})(\eta^{1/2}+\delta)+\nu_2(\mu_1+\mu_2\xi^{-1/4})]$ $-(\eta^{1/2}-\delta)^{-4}z^{-2}[\nu_1\eta^{-1/4}(\eta^{1/2}+\delta)+\nu_2]^2$
(IV) $\alpha^2z^{-2/3}+\beta^2\bar{z}^{-2/3}+\mu_1\xi^{-1/3}+\mu_2\xi^{-2/3}+\xi^{-1}\eta^{1/3}[\nu_1(\eta^{1/3}-\delta)^{-2}+\nu_2(\eta^{1/3}+\delta)^{-2}]$	$\frac{1}{2}(-3A'+B'+C+\xi^{-1}D)z^2p_z^2+(A'+B'-C-3\xi^{-1}D)\xi p_zp_{\bar{z}}+\frac{1}{2}(A'-3B'+C$ $+\xi^{-1}D)\bar{z}^2p_{\bar{z}}^2+\mu_2(\alpha^2\eta^{1/3}+\beta^2\eta^{-1/3})+z\bar{z}^{-1/3}(\alpha^2\eta^{2/3}-\beta^2)^2-[\mu_1(\nu_1+\nu_2)$ $-2\alpha\beta(\nu_1-\nu_2)]\bar{z}^{-2/3}+\nu_1(\eta^{1/3}-\delta)^{-2}[(2\beta^2-\mu_1\delta)(2\xi^{-1/3}-\delta\bar{z}^{-2/3})$ $-\mu_2z^{-1}\bar{z}^{-1/3}]+\mu_2(\eta^{1/3}+\delta)^{-2}[(2\beta^2+\mu_1\delta)(2\xi^{-1/3}+\delta\bar{z}^{-2/3})-\mu_2z^{-1}\bar{z}^{-1/3}]$
$\delta=\beta/\alpha$	$-z^{-5/3}\bar{z}^{-1/3}[\nu_1(\eta^{1/3}-\delta)^{-2}+\nu_2(\eta^{1/3}+\delta)^{-2}]^2$

where $\delta=\beta/\alpha$,

$$\text{(IV)}\quad V(z,\bar{z})=\alpha^2 z^{-2/3}+\beta^2\bar{z}^{-2/3}+\mu_1\xi^{-1/3}+\mu_2\xi^{-2/3}+\xi^{-1}\eta^{1/3}[\nu_1(\eta^{1/3}-\delta)^{-2}+\nu_2(\eta^{1/3}+\delta)^{-2}], \tag{4.12}$$

where $\delta=\beta/\alpha$, along with those obtained by $z\leftrightarrow\bar{z}$.

To complete the determination of the invariant, the equations in (4.3) must be integrated to find c_{00} for each of the potentials. The potentials together with their invariants are listed in Table I. With α and β equal to 0, the quartic invariants reduce to products of a quadratic invariant and the Hamiltonian.

Now some comments may be made on the nature of the potentials. All the integrable potentials constructed here (including the one in the previous section) are discontinuous along the positive real axis because of terms like $\bar{z}^{-1/2}$, etc. Potentials I and II in (4.12) are complex valued for all choices of β. Potential III is real valued under either of the following choices: (i) $\alpha=\beta$ and all coefficients are real; (ii) $\beta=\alpha^*$ and $\nu_1^2/\nu_1^{*2}=\nu_2/\nu_2^*=\alpha^{*2}/\alpha^2$; μ_1, μ_2 are real. Potential IV is real valued under either of the following choices: (i) $\alpha=\beta$ and all coefficients are real; (ii) $\beta=\alpha^*$ and $\nu_1/\nu_1^*=\nu_2/\nu_2^*=\alpha^{*2}/\alpha^2$; μ_1, μ_2 are real.

Potential III can be considered as an extension of the potential in (3.14) which itself was an extension of the Kepler potential. Do there exist extensions of these potentials with invariants at higher order? At fifth and sixth order, with power law solutions for $A(z)$ and $B(\bar{z})$, no integrable potentials exist. Such is likely to be the case at higher orders as well. Thus there would appear to be no extensions to (3.14) and (4.11) along the lines considered here. With A and B set to 0, the solution (2.17) of the linear PDE for the potential reduces to

$$V=C(z\bar{z})+\sum_{k=2}^{n-2}\frac{1}{(z\bar{z})^{k/2}}D_k\left(\frac{\bar{z}}{z}\right)\equiv F(r)+\sum_{k=0}^{n-4}\frac{1}{r^{k+2}}G_k(\theta). \tag{4.13}$$

It has been found (Sen[11]) that this is precisely the necessary general form of a potential for it to admit an invariant of the form given in (2.5) but of order $(n-2)$. Thus if the potential is not to admit a lower order invariant both A and B must not vanish. The possibility of solutions other than power law for $A(z)$ [or $B(\bar{z})$] at fifth and sixth order has not been investigated. Even at fourth order our results are incomplete and there might well exist other solutions to (4.7) besides those found here. The complexity of the forms of $f(z)$, $g(\bar{z})$, and $h(z,\bar{z})$ in (4.8) would appear to indicate that construction of other solutions may not be straightforward. It should also be noted that the quantum integrability of the potentials in (4.12) is not assured but must be checked for each case by computing the Moyal bracket of I and H. However, that question is not considered here.

At this stage one might well question the utility of constructing invariants at high orders. Certainly from a practical point of view, the behavior (in say, configuration space) of an integrable potential with a high-order invariant might appear to be little different from that of a nonintegrable potential. However, the existence of the invariant permits one to make global statements about the system. For instance, if the motion is bounded and a periodic solution is known to exist, then there must in fact be a one-parameter (or $d-1$ parameter for d-dimensional integrable systems) family of periodic solutions. Moreover, many systems can be approximated by integrable ones and it is useful to understand the kinds of behavior exhibited by a variety of integrable systems. If one's interest is more in the mathematical question of what determines integrability, then explicit examples of integrable potentials can be used to test any proposed integrability criteria. We do precisely this in the next section.

V. PAINLEVÉ ANALYSIS

The original conjecture that integrable systems should possess the Painlevé property, i.e., their only movable singularities in the complex time plane must be poles, was made by Ablowitz, Ramani, and Segur[22] for nonlinear partial differential equations. This has been extended to discrete dynamical systems and has proved to be useful in identifying various integrable cases.[6] There is, however, no general proof as of yet that integrable systems must satisfy this property and the relation between this analytic property and the existence of an invariant is still unclear. In this section the integrable potentials constructed in the previous two sections are tested for this property,

$$V=\alpha z^{-1/2}+\beta\bar{z}^{-1/2}+\gamma(z\bar{z})^{-1/2}. \tag{5.1}$$

This is the potential in (3.14). The second-order equations of motion are

$$\ddot{z}=\beta\bar{z}^{-3/2}+\gamma z^{-1/2}\bar{z}^{-3/2},\quad \ddot{\bar{z}}=\alpha z^{-3/2}+\gamma z^{-3/2}\bar{z}^{-1/2}. \tag{5.2}$$

Assume that the dominant behavior of z and $\bar{z}$ as $\tau=(t-t_0)\to 0$ is $z\sim a\tau^p$, $\bar{z}\sim b\tau^q$. Balancing the most singular terms, one finds the two possibilities: (i) $p=q=\frac{4}{5}$. The resonances are $r=-1,\frac{2}{5},-\frac{1}{5},-\frac{2}{5}$; (ii) $p=q=\frac{2}{3}$. The resonances are $r=0,-1,\frac{2}{3},-\frac{1}{3}$.

Besides -1,0 the other values of r should be positive in order to get the complete four-parameter solution. Since that does not hold in either case, the leading order behaviors obtained above cannot describe the general solution. However, we know that for this potential, the Hamilton–Jacobi equation separates in parabolic coordinates leading to two one-dimensional problems. The trajectories can be obtained exactly. This was done by Winternitz *et al.*[15] and we quote their result (for the real potential $\beta=\alpha^*$),

$$\zeta_i=\frac{\kappa_i}{2E}+\left(\frac{\kappa_i^2}{4E^2}-\frac{a_i}{E}\right)^{1/2}\sin\left(\sqrt{-2E}\,\tau+b_i\right),\quad i=1,2, \tag{5.3}$$

where ζ_i are the parabolic coordinates, E is the energy, τ is a time parameter, and $\kappa_1=\alpha+\alpha^*$, $\kappa_2=i(\alpha^*-\alpha)$. Here a_i, b_i are the four arbitrary parameters. Clearly this does not show any singular behavior.

Now consider the potentials with quartic invariants giv-

en in (4.12), in order,

$$V=\beta\bar{z}^{-1/2}+\mu_1\xi^{-1/2}+\mu_2\xi^{-3/2}+\xi^{-1}(\nu_1\eta^{1/4}+\nu_2\eta^{1/2}). \tag{5.4}$$

The equations of motion are

$$\begin{aligned}\ddot{z}&=\beta\bar{z}^{-3/2}+\mu_1 z^{-1/2}\bar{z}^{-3/2}+\tfrac{3}{2}\mu_2 z^{-3/4}\bar{z}^{-7/4}\\&\quad+\tfrac{3}{2}\nu_1 z^{-5/4}\bar{z}^{-7/4}+\nu_2 z^{-3/2}\bar{z}^{-3/2},\\\ddot{\bar{z}}&=\mu_1 z^{-3/2}\bar{z}^{-1/2}+\tfrac{3}{2}\mu_2 z^{-7/4}\bar{z}^{-3/4}+\tfrac{5}{2}\nu_1 z^{-9/4}\bar{z}^{-3/4}\\&\quad+3\nu_2 z^{-5/2}\bar{z}^{-1/2}.\end{aligned} \tag{5.5}$$

Assuming $z\sim a\tau^p$, $\bar{z}\sim b\tau^q$ as $\tau=(t-t_0)\to 0$, we have the following possibilities: (1) $p=q=\frac{1}{2}$. The resonances are $r=-\frac{1}{4},-1,1,\frac{1}{4}$. This gives a three-parameter solution. (ii) $p=2=-q$. The resonances are $r=-1,0,1,2$. This gives a four-parameter solution. (iii) $p=-3$, $q=5$. The resonances are $r=-2,-1,0,1$. This gives a three-parameter solution. Thus only (ii) can describe the general solution. The expansions for $z,\bar{z}$ read

$$z=a\tau^2+\cdots,\quad \bar{z}=(\nu_2/2)^{2/3}a^{-5/3}\tau^{-2}+\cdots. \tag{5.6}$$

Potential (II) in (4.12) shows similar behavior. Now consider potential (III),

$$\begin{aligned}V(z,\bar{z})&=\alpha z^{-1/2}+\beta\bar{z}^{-1/2}+\mu_1\xi^{-1/2}+\mu_2\xi^{-3/4}\\&\quad+\xi^{-1}(\eta^{1/2}-\delta)^{-2}[\nu_1\eta^{1/4}(\eta^{1/2}+\delta)\\&\quad+\nu_2\eta^{1/2}],\end{aligned} \tag{5.7}$$

where $\delta=\beta/\alpha$. It was remarked earlier in Sec. IV that this potential can be considered as an extension of the potential in (3.14) and indeed the singularity analysis shows similar behavior. The equations of motion for this potential are

$$\begin{aligned}\ddot{z}&=\beta\bar{z}^{-3/2}+\mu_1 z^{-1/2}\bar{z}^{-3/2}+\tfrac{3}{2}\mu_2 z^{-3/4}\bar{z}^{-7/4}\\&\quad+(z^{-1/2}\bar{z}^{1/2}-\delta)^{-3}\big[\tfrac{5}{2}\nu_1 z^{-9/4}\bar{z}^{-3/4}+3\nu_2 z^{-2}\bar{z}^{-1}\\&\quad+\delta(3\nu_1 z^{-7/4}\bar{z}^{-5/4}-\nu_2 z^{-3/2}\bar{z}^{-3/2}\\&\quad-\tfrac{3}{2}\delta\nu_1 z^{-5/4}\bar{z}^{-7/4})\big],\\\ddot{\bar{z}}&=\alpha z^{-3/2}+\mu_1 z^{-3/2}\bar{z}^{-1/2}+\tfrac{3}{2}\mu_2 z^{-7/4}\bar{z}^{-3/4}\\&\quad+(z^{-1/2}\bar{z}^{1/2}-\delta)^{-3}\big[\tfrac{3}{2}\nu_1 z^{-13/4}\bar{z}^{1/4}+\nu_2 z^{-3}\\&\quad-\delta(3\nu_1 z^{-11/4}\bar{z}^{-1/4}+3\nu_2 z^{-5/2}\bar{z}^{-1/2}\\&\quad+\tfrac{5}{2}\delta\nu_1 z^{-9/4}\bar{z}^{-3/4})\big].\end{aligned} \tag{5.8}$$

With $z\sim a\tau^p$, $\bar{z}\sim b\tau^q$, none of the various possibilities for p and q give a four-parameter solution. The most we get are the three-parameter solutions with either (i) $p=5$, $q=-3$. Resonances are $r=-2,-1,0,1$; (ii) $p=-3$, $q=5$. The same resonances as above.

We argue that the leading order behavior is not expected to be singular because of the following reason. For $p=5$, $q=-3$ the most singular terms on the right-hand sides of (5.8) arise from the term $\nu_1 z^{-3/4}\bar{z}^{-5/4}$ in the potential (5.7). Now $z^{-3/4}\bar{z}^{-5/4}=r^{-2}e^{i\theta/2}$, where (r,θ) are the polar coordinates. With a potential of the form $V=r^{-2}f(\theta)$ the Hamilton–Jacobi equation separates and the coordinates are expressible in terms of periodic functions of time. A similar argument holds for case (ii). Thus the potential (called here the second extension of the Kepler potential) shows similar nonsingular behavior as the potential in (5.1) (the first extension of the Kepler potential).

Potential (IV) in (4.12) shows similar nonsingular behavior as the previous one. Thus it is seen that the equations of motion for the integrable potentials constructed in Sec. III and IV either do not exhibit nonsingular behavior or else have the Painlevé property.

VI. CONCLUDING REMARKS

In this work we have constructed examples of two-dimensional integrable Hamiltonian systems which admit an invariant of the chosen form (2.7). The potential in (3.14) reveals itself to be a close relative of the Kepler potential. Under the same time transformation which turns the Kepler potential into the harmonic oscillator in parabolic coordinates, the system (3.14) is transformed into the harmonic oscillator acted on by a constant force. The system (3.14) is also superintegrable and its invariants provide a representation of the Lie algebra sO(3) for negative energies and sO(2,1) for positive energies. Unlike the Kepler potential however, its equations of motion do not admit any finite symmetries. The potentials in (4.12) admit a quartic invariant of the form (2.7) and of them, potential (III) can be considered as an extension of (3.14). Recently it was shown by Yoshida[23] that potentials of the form

$$V=a/r+bx^n+cy^n, \tag{6.1}$$

where a,b,c,n are constants are integrable only if (i) $n=1$, b,c arbitrary, (ii) $n=2$, $b=c$, and (iii) $n=2$, $b=4c$ (or $c=4b$). Other perturbations to the Kepler potential of this form do not lead to an integrable system. In this context one may view (3.14) and potential III in (4.12) as perturbations of the Kepler potential which do preserve integrability. One should bear in mind that all potentials of the form

$$V=a/r+(1/r^2)f(\theta), \tag{6.2}$$

where f is an arbitrary function, are integrable and admit a quadratic invariant. In other words, the Kepler system may also remain integrable under a whole class of perturbations unlike the cases mentioned above where integrability is preserved with only specific perturbations.

The analytic structure of the integrable systems constructed here has been studied and it was found that they either do not show singular behavior or else their movable singularities are indeed poles, thus verifying the Painlevé conjecture.

Let us indicate possible extensions to this work. Using (2.3) we can rewrite the general form (2.2) of an invariant as

$$\begin{aligned}I&=C_{00}^n L^n+(C_{10}^{n-1}p_x+C_{01}^{n-1}p_y)L^{n-1}\\&\quad+(C_{20}^{n-2}p_x^2+C_{11}^{n-2}p_x p_y+C_{02}^{n-2}p_y^2)L^{n-2}+\cdots\\&\quad+C_{n0}^0 p_x^n+C_{n-11}^0 p_x^{n-1}p_y+\cdots+C_{0n}^0 p_y^n\\&\quad+\text{lower-order terms in the momenta},\end{aligned} \tag{6.3}$$

where C_{ij}^k are constants and $L=xp_y-yp_x$. In this work we took $C_{20}^{n-2}=1=C_{02}^{n-2}$ and all others 0 while in Sen,[11] invariants with $C_{00}^n=1$ and all other constants 0 have been studied. Clearly one must try to establish similar results or show the nonexistence of integrable potentials for other

choices of coefficients. In addition to polynomial invariants, Darboux's method can also be used[4] to treat invariants which are rational or transcendental in the momenta. This extension needs to be studied in depth.

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APPENDIX: LIE SYMMETRIES OF (3.14)

Prince and Eliezer[24] have shown that the Kepler potential admits three point Lie symmetry generators. They also claim that as a consequence the Runge–Lenz vector is conserved but this has been disputed.[25] We follow the notation of Prince and Eliezer and show that the system (3.14) (the first extension of the Kepler system) admits only the trivial time translation generator.

A system of second-order differential equations,

$$\mathbf{F}(t,\mathbf{x},\dot{\mathbf{x}},\ddot{\mathbf{x}})=0, \tag{A1}$$

admits a point Lie symmetry if it is invariant under the infinitesimal point transformations

$$t'=t+\epsilon\xi(\mathbf{x},t),\quad x_i'=x_i+\epsilon\eta_i(\mathbf{x},t) \tag{A2}$$

(ϵ is an infinitesimal parameter) generated by the operator

$$U=\xi(\mathbf{x},t)\partial_t+\eta_i(\mathbf{x},t)\partial_{x_i}. \tag{A3}$$

The condition of invariance is

$$U''\mathbf{F}=0, \tag{A4}$$

where U'' is the twice extended operator

$$U''=\xi\partial_t+\eta_i\partial_{x_i}+\eta_i'\partial_{\dot{x}_i}+\eta_i''\partial_{\ddot{x}_i}, \tag{A5}$$

with

$$\eta_i^k(\mathbf{x},\dot{\mathbf{x}},\ldots,\mathbf{x}^{(k)},t)\equiv\frac{d}{dt}\eta_i^{k-1}-x_i^{(k)}\frac{d}{dt}\xi, \tag{A6}$$

where $\mathbf{x}^{(k)}\equiv(d^k/dt^k)\mathbf{x}$. The equations of motion for the system (3.14) are

$$\ddot{z}=\beta\bar{z}^{-3/2}+\gamma z^{-1/2}\bar{z}^{-3/2},\quad \ddot{\bar{z}}=\alpha z^{-3/2}+\gamma z^{-3/2}\bar{z}^{-1/2}. \tag{A7}$$

The infinitesimal symmetry generator is

$$U=\xi(z,\bar{z},t)\partial_t+\eta_1(z,\bar{z},t)\partial_z+\eta_2(z,\bar{z},t)\partial_{\bar{z}}, \tag{A8}$$

and its twice extended form is

$$U''=\xi\partial_t+\eta_1\partial_z+\eta_2\partial_{\bar{z}}+(\dot{\eta}_1-\dot{z}\dot{\xi})\partial_{\dot{z}}+(\dot{\eta}_2-\dot{\bar{z}}\dot{\xi})\partial_{\dot{\bar{z}}}+(\ddot{\eta}_1-2\ddot{z}\dot{\xi}-\dot{z}\ddot{\xi})\partial_{\ddot{z}}+(\ddot{\eta}_2-2\ddot{\bar{z}}\dot{\xi}-\dot{\bar{z}}\ddot{\xi})\partial_{\ddot{\bar{z}}}. \tag{A9}$$

Applying this to (A7) and equating the coefficients of different powers of $\dot{z}$, $\dot{\bar{z}}$ to 0, we get ($\xi_{,zz}\equiv\partial_z^2\xi$, etc.),

$$\xi_{,zz}=0;\quad \xi_{,z\bar{z}}=0;\quad \xi_{,\bar{z}\bar{z}}=0, \tag{A10}$$

$$\eta_{1,zz}=2\xi_{,zt};\quad \eta_{1,z\bar{z}}=\xi_{,\bar{z}t};\quad \eta_{1,\bar{z}\bar{z}}=0, \tag{A11}$$

$$\eta_{2,zz}=0;\quad \eta_{2,z\bar{z}}=\xi_{,zt};\quad \eta_{2,\bar{z}\bar{z}}=2\xi_{,\bar{z}t},\quad 2\eta_{1,zt}=3(\beta\bar{z}^{-3/2}+\gamma z^{-1/2}\bar{z}^{-3/2})\xi_{,z}+(\alpha z^{-3/2}+\gamma z^{-3/2}\bar{z}^{-1/2})\xi_{,\bar{z}}+\xi_{,tt},$$
$$\eta_{1,\bar{z}t}=(\beta\bar{z}^{-3/2}+\gamma z^{-1/2}\bar{z}^{-3/2})\xi_{,\bar{z}},\quad \eta_{2,zt}=(\alpha z^{-3/2}+\gamma z^{-3/2}\bar{z}^{-1/2})\xi_{,z},$$
$$2\eta_{2,\bar{z}t}=(\beta\bar{z}^{-3/2}+\gamma z^{-1/2}\bar{z}^{-3/2})\xi_{,z}+3(\alpha z^{-3/2}+\gamma z^{-3/2}\bar{z}^{-1/2})\xi_{,\bar{z}}+\xi_{,tt}, \tag{A12}$$

$$\eta_{1,z}(\beta\bar{z}^{-3/2}+\gamma z^{-1/2}\bar{z}^{-3/2})+\eta_{1,\bar{z}}(\alpha z^{-3/2}+\gamma z^{-3/2}\bar{z}^{-1/2})+\eta_{1,tt}+\tfrac{1}{2}\eta_1\gamma(z\bar{z})^{-3/2}$$
$$+\tfrac{3}{2}\eta_2(\beta\bar{z}^{-5/2}+\gamma z^{-1/2}\bar{z}^{-5/2})-2(\beta\bar{z}^{-3/2}+\gamma z^{-1/2}\bar{z}^{-3/2})\xi_{,t}=0,$$

$$\eta_{2,z}(\beta\bar{z}^{-3/2}+\gamma z^{-1/2}\bar{z}^{-3/2})+\eta_{2,\bar{z}}(\alpha z^{-3/2}+\gamma z^{-3/2}\bar{z}^{-1/2})+\eta_{2,tt}+\tfrac{1}{2}\eta_2\gamma(z\bar{z})^{-3/2}$$
$$+\tfrac{3}{2}\eta_1(\alpha z^{-5/2}+\gamma z^{-5/2}\bar{z}^{-1/2})-2(\alpha z^{-3/2}+\gamma z^{-3/2}\bar{z}^{-1/2})\xi_{,t}=0. \tag{A13}$$

It is straightforward to check that the only solution of these equations when $\alpha\neq0\neq\beta$ is

$$\xi=\text{const},\ \eta_1=0=\eta_2, \tag{A14}$$

giving the Lie symmetry generator

$$U=\partial_t. \tag{A15}$$

This time translation symmetry that exists for all time-independent potentials is associated only with the conservation of energy. The importance of Lie symmetries arises by virtue of Lie's theorem that the infinitesimal point transformations can be integrated to give a finite continuous group of transformations. This is usually not the case for other kinds of local symmetries. The lack of any finite space-time symmetry transformations for this completely degenerate potential shows that there is no direct connection between such symmetries and degeneracy.

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where a, b, m are constants, for which (3.8) is not satisfied. However, this solution leads to a spherically symmetric potential. I consider only the ansatz (3.8) here since this is the only one to have led to a nonspherically symmetric potential. I thank Jacques Perk for suggesting the transformation which converts (3.6) to an autonomous equation and for pointing out the above solution.

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Second-order equation fields and the inverse problem of Lagrangian dynamics

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The transformation properties of determined, autonomous systems of second-order ordinary differential equations, identified as vector fields on the tangent bundle of the space of dependent variables, are derived and studied. The inverse problem of Lagrangian dynamics is studied from this transformation viewpoint as well as the problem of alternative Lagrangians. In particular, regular Lagrangians which are analytic as functions of the first derivatives are considered. Finally, the inverse problem for second-order systems corresponding to the geodesic flow of a symmetric linear connection is investigated.

I. INTRODUCTION

The inverse problem of Lagrangian dynamics asks for necessary and sufficient conditions that a given system of second-order ordinary differential equations are the Euler–Lagrange equations corresponding to a regular Lagrangian function. Allied to the inverse problem is the question of when two Lagrangian functions, which are not trivially equivalent (a term which will be explained in Sec. III), determine the same second-order system, the so-called problem of alternative Lagrangians. There has been a certain amount of progress made recently in answering these important questions, which have all sorts of theoretical and practical ramifications, but a complete solution is, for the moment at least, not in sight.

The main aim of this paper is to make a thorough study of the transformation properties of systems of autonomous second-order ordinary differential equations and apply the results obtained to the inverse problem. For the sake of simplicity, throughout this paper I shall only consider autonomous systems, though for the most part this is not an essential restriction. In Sec. II I consider the correspondence between such systems and certain kinds of vector fields known as second-order equation fields. This correspondence leads in a natural way to a "transformation law" for second-order systems, several simple consequences of which are presented. The material of Sec. II (and Sec. III) is not intended to be simply an exercise in mathematical erudition: a modern approach to a system of differential equations (even in the context of Euclidean space) is to consider two such systems as being equivalent, if one can be transformed into the other using a change of coordinates belonging to some specified pseudogroup of coordinate transformations. This pseudogroup is chosen at the outset and is dictated by the significance attached to the independent and dependent variables. A set of differential equations then is more properly regarded as an equivalence class of systems, any two representatives of the class being related by a coordinate transformation of the given pseudogroup.

The other theme of the paper, in Secs. III–V, is a study of a restricted class of second-order equation fields, namely, those corresponding to second-order systems analytic in the first derivatives. In particular, the inverse problem for such systems is investigated. In Sec. III the inverse problem is introduced and some basic points concerning it are made. In Sec. IV some simple consequences of a direct approach to the inverse problem are derived. This approach is an alternative to the Helmholtz equations which provide necessary and sufficient conditions for the existence of a regular Lagrangian, whose Euler–Lagrange field is the given second-order equation field.[1,2] In Sec. V I consider the inverse problem for second-order equation fields which are the geodesic sprays of symmetric linear connections. It is shown that the conditions for the existence of a Lagrangian have a simple geometric interpretation. These conditions are used to exhibit several examples of sprays which admit alternative Lagrangians.

Sections II and III employ some geometric machinery of the tangent bundle, a comprehensive treatment of which can be found in Crampin,[3] whereas Secs. IV and V are analytical in character. As regards notation, M consistently denotes a "smooth," that is class C^∞, manifold. The tangent bundle submersions from TM to M and TTM to TM will be denoted by π and Π, respectively, and the tangent mapping of π from TTM to TM is denoted by $T\pi$. The second-order tangent bundle to M, that is, equivalence classes of (germs of) curves on M which agree to second order, is denoted by T^2M. If (x^i) is a system of local coordinates on M, there is a naturally induced system (x^i, u^i) on TM which I refer to as an adapted coordinate system. Similarly (x^i,u^i,y^i,v^i) denotes a coordinate system on TTM induced from (x^i, u^i) on TM. The notation of classical tensor calculus is used with a repeated index denoting summation. For a (covariant) tensor field of valence n whose components are $A_{i_1\cdots i_n}$, its symmetric part is denoted by $A_{(i_1\cdots i_n)}$.

Finally, I mention two lifting constructions on the tangent bundle. First, a one-form α on M defines in a natural way a real-valued function on TM, denoted by $\tilde{\alpha}$. If $u\in TM$ and $\pi(u) = x$, $\tilde{\alpha}(u)$ is defined as the result of pairing u with $\alpha(x)$ (as elements of T_xM and T^*_xM, respectively). In an adapted coordinate system (x^i, u^i) on TM if locally α is represented by $\alpha_i\, dx^i$, $\tilde{\alpha}$ is given locally by $(x^i, u^i)\mapsto\alpha_i u^i$. Second, if A is a tensor field on M of type $(1, n)$ which is symmetric in its covariant arguments, it determines naturally a vertical vector field on TM written A^v. If (x^i, u^i) is an adapted coordinate system and A is represented locally by

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$A^{j}_{i_1}\cdots_{i_n}(\partial/x^j)\otimes dx^{i_1}\,dx^{i_2}\cdots dx^{i_n}$, A^{v} is given locally by $A^{j}_{i_1}\cdots_{i_n}u^{i_1}u^{i_2}\cdots u^{i_n}(\partial/\partial u^j)$. This vertical lift construction is the natural generalization of the usual vertical lift construction in which a vector field on M is lifted to a vertical field on TM which is "constant on fibers."[3,4]

II. FOUNDATIONAL REMARKS ON SECOND-ORDER EQUATIONS

A second-order equation field (SOEF) Γ on an m-dimensional manifold M is a section of TTM over TM with respect to both the submersion maps $T\pi$ and Π. In other words, Γ is a vector field on TM such that for all u in TM,

$$(\pi_*\Gamma)_u = u. \tag{2.1}$$

A SOEF provides a convenient geometric description of a regular, determined, autonomous system of second-order ordinary differential equations. To say the system is "determined" is to say that there are as many independent equations as there are dependent variables and by "regularity" I mean that the second-order derivatives can always be solved for as functions of the first-order derivatives and dependent variables. If (x^i, u^i) is a local coordinate system on TM adapted to the tangent bundle fibration, Γ assumes the form

$$\Gamma = u^i\frac{\partial}{\partial x^i} + f^i\frac{\partial}{\partial u^i}, \tag{2.2}$$

where the f^i's are functions of x^i and u^i. The second-order system corresponding to Γ is given by

$$\ddot{x}^i = f^i(x^j, \dot{x}^j), \tag{2.3}$$

where the dot denotes differentiation with respect to the independent variable t. Setting $u^i = \dot{x}^i$ is the well-known device which effectively converts (2.3) into (2.2).

The second-order system (2.3) is amenable to a somewhat different geometric interpretation which at once explains the significance of the regularity condition and enables one to interpret (2.3) in terms of the second-order tangent bundle T^2M. In fact consider T^2M as a bundle over TM. (One should note carefully that T^2M naturally has the structure of an affine rather than a vector bundle over TM; for more about affine bundles see Crampin and Thompson.[5]) If (x^i, u^i, v^i) is an adapted coordinate system on T^2M, then one may consider (2.3) as defining (locally) a codimension m submanifold, Σ say, of T^2M by the conditions

$$v^i = f^i(x^j, u^j)\ . \tag{2.4}$$

In fact Σ actually defines a section σ of T^2M over TM and thus may be identified with TM. Notice that it is precisely the regularity condition which guarantees that Σ defines a section of T^2M over TM.

I shall explain next how the considerations of the previous paragraph lead naturally to the definition of a SOEF as given above starting from the second-order system (2.3). Note first of all that T^2M is naturally an embedded submanifold of TTM. If (x^i, u^i, y^i, v^i) is a coordinate system on TTM consonant with the adapted coordinate system (x^i, u^i, y^i, v^i) on T^2M, T^2M is locally the submanifold given by the conditions $u^i = y^i$. Let the submanifold map from T^2M to TTM be denoted by j. Notice that $j(T^2M)$ is invariant under the action of the canonical involution I on TTM. It follows that the map $j\circ\sigma$ defines a section of TTM over TM with respect to both the submersion maps $T\pi$ and Π, in other words is a SOEF on M.

I next introduce the notion of isomorphism SOEF's, which makes the collection of SOEF's on manifolds diffeomorphic to a fixed manifold into a groupoid. Suppose that Γ_1 and Γ_2 are SOEF's on M_1 and M_2, respectively. Then Γ_1 and Γ_2 [or more accurately (Γ_1, M_1) and (Γ_2, M_2)] are isomorphic or equivalent, if there exists a diffeomorphism ϕ of M_1 with M_2 such that at each point of TM_1,

$$(T\phi)_*\Gamma_1 = \Gamma_2. \tag{2.5}$$

Equation (2.5) enables us to define what it means for two second-order systems to be equivalent (at least second-order systems corresponding to SOEF's). It is important to appreciate that this is the appropriate categorical meaning of equivalence of second-order systems; one could envisage other notions of equivalence, but these will either destroy some property which is characteristic of such systems or preserve some uncharacteristic property.

We can ask what (2.5) means locally. To this end, let $(\bar{x}^i, \bar{u}^i)$, $(\bar{x}^i, \bar{u}^i)$ be two adapted coordinate systems on TM_1 and TM_2, respectively, and suppose that

$$\Gamma_1 = u^i\frac{\partial}{\partial x^i} + f^i\frac{\partial}{\partial u^i}, \tag{2.6}$$

$$\Gamma_2 = \bar{u}^i\frac{\partial}{\partial \bar{x}^i} + \bar{f}^i\frac{\partial}{\partial \bar{u}^i}. \tag{2.7}$$

If now the transformation $T\phi$ is described locally by

$$\bar{x}^i = \bar{x}^i(x^j)\ , \tag{2.8}$$

$$\bar{u}^i = \frac{\partial \bar{x}^i}{\partial x^j}u^j, \tag{2.9}$$

we find (2.5) gives the following transformation law of second-order equations:

$$\bar{f}^i = f^a\frac{\partial \bar{x}^i}{\partial x^a} + \bar{u}^a\bar{u}^b\frac{\partial^2\bar{x}^i}{\partial x^c\partial x^e}\frac{\partial x^c}{\partial \bar{x}^a}\frac{\partial x^e}{\partial \bar{x}^b}. \tag{2.10}$$

Equation (2.10) may be interpreted in the spirit of classical tensor analysis; it says, assuming that Γ_1 and Γ_2 are analytic in the fiber u, that every term transforms tensorially, except the quadratic one, which transforms according to the transformation law for Christoffel symbols. Thus, for $n\neq 2$, the term of degree n in f^a, $A^{a}_{j_1\cdots j_n}u^{j_1}\cdots u^{j_n}$ say, arises from the type $(1,n)$ tensor field $A^{a}_{j_1\cdots j_n}$ on M and $A^{a}_{j_1\cdots j_n}u^{j_1}\cdots u^{j_n}(\partial/\partial u^a)$ is just its vertical lift in the sense of Sec. I. We can therefore decompose a given SOEF Γ, which is analytic in u, into a sum of a spray together with various vector fields which are vertical lifts. Thus I shall write

$$\Gamma = \Lambda + A^{V}_{0} + A^{V}_{1} + A^{V}_{3} + A^{V}_{4} + \cdots, \tag{2.11}$$

where Λ is the spray associated to Γ and A^{V}_{n} is the vertical lift field corresponding to the terms of degree n in u and which is invariantly associated to Γ. It is worth noting too that the notion of a spray, which is by definition a SOEF in which the f^i's are homogeneous quadratic polynomials in u^j, is well defined in virtue of (2.10); this is not obvious *a priori*.

I shall present next some applications of (2.5). I shall make use of the well-known result in connection theory

which asserts that if the curvature of a torsion-free (linear) connection vanishes, one can always introduce local coordinates relative to which the Christoffel symbols of the connection are zero.[6,7]

Proposition 2.1: Suppose that Γ_1 and Γ_2 are two SOEF's analytic in the fiber variables. Suppose further, that Γ_1 has a nonzero term of degree n ($\neq 2$) in u but that Γ_2 does not. Then Γ_1 and Γ_2 are not equivalent.

Proposition 2.2: Suppose we are given a second-order system of type (2.3) with corresponding SOEF Γ. Then we can find a local representation as

$$\ddot{\bar{x}}^i = \bar{f}^i(\bar{x}^j) \tag{2.12}$$

iff (i) $\Gamma = \Lambda + A_0^V$, that is, the f^i's are even quadratic in u, and (ii) the curvature of the connection corresponding to Λ vanishes.

Proposition 2.3: Suppose we are given a second-order system of type (2.3) with corresponding SOEF Γ. Then we can find a linear representation

$$\ddot{\bar{x}}^i = A^i + B^i_j \bar{x}^j + C^i_j \ddot{\bar{x}}^j, \tag{2.13}$$

where A^i is a constant m vector and B^i_j and C^i_j are constant $m \times m$ matrices iff (i) $\Gamma = \Lambda + A_0^V + A_1^V$, that is, the f^i's are quadratic in u; (ii) the curvature of the connection ∇ corresponding to Λ vanishes; and (iii) $\nabla A_1 = 0$ and $\nabla^2 A_0 = 0$.

Condition (ii) says that we can remove the term quadratic in u and thereafter, according to (2.10), we must only consider transformations which are affine linear in x. (Any other transformation would reintroduce terms quadratic in u.) Condition (iii) then guarantees that the term of degree 0 in u is affine linear in x.

Thus for autonomous systems of second-order ordinary differential equations there is a complete characterization of those systems that are equivalent to linear systems. Moreover, this characterization yields an effective practical test for determining whether a given second-order system can be linearized. This is in stark contrast to the situation for even scalar nonautonomous second-order equations. (See Ref. 8 for some recent results on this subject.)

III. THE INVERSE PROBLEM OF LAGRANGIAN DYNAMICS

In this section I shall briefly review the geometrical approach to Lagrangian dynamics and describe the inverse problem in the light of the material of Sec. II. This is intended to put the inverse problem into some kind of perspective, prior to the more specific analysis in Secs. IV and V.

To formulate Lagrangian theory invariantly, we shall have to investigate the geometry of the tangent bundle TM in greater detail. In particular we shall need the canonical Liouville vector Δ and the 1–1 tensor field S, the so-called vertical endomorphism. The vector field Δ arises out of the action of the multiplication group of nonzero reals on each fiber of TM; specifically, if F is any real-valued function on TM and u an arbitrary point in TM,

$$(\Delta F)(u) = \frac{d}{dt}(F(tu))\Big|_{t=0}. \tag{3.1}$$

The tensor S is defined as follows. Let $u \in TM$ and $X \in T_u(TM)$; then $S(X)_u$ is $\Delta(\pi_* X)$, which makes sense because $\pi_* X$ is an element of TM. In an adapted coordinate system (x^i, u^i) on TM, Δ and S assume the form $u^i(\partial/\partial u^i)$ and $(\partial/\partial u^i) \otimes dx^i$, respectively.

Now suppose that L: $TM \to \mathbf{R}$ is a regular Lagrangian. This means that in the adapted coordinates (x^i, u^i),

$$\det\left(\frac{\partial^2 L}{\partial u^i \partial u^j}\right) \neq 0. \tag{3.2}$$

Now since S is a 1–1 tensor, it can be applied to the one-form dL to produce another one-form $S \circ dL$. It follows from (3.2) that the two-form $\omega_L = d(S \circ dL)$ is a symplectic form. The Euler–Lagrange field Λ determined by L is the unique vector field which satisfies

$$i(\Lambda)\omega_L = -d(\Delta L - L). \tag{3.3}$$

One may readily check that Λ so defined is indeed a SOEF on M. The inverse problem of Lagrangian dynamics asks for necessary and sufficient conditions that a given SOEF is the Euler–Lagrange field corresponding to some regular Lagrangian function on TM. For more on the invariant formulation of Lagrangian dynamics the reader can refer to Refs. 3, 9, and 10.

Now consider all pairs $(\bar{M}, \bar{L})$ consisting of a manifold $\bar{M}$ diffeomorphic to M and a regular Lagrangian function $\bar{L}$ on $T\bar{M}$. The collection of all such pairs forms a category, indeed groupoid, in the obvious way. We can now describe the assignment of a SOEF corresponding to a regular Lagrangian as a functor $\mathcal{F}$ from this groupoid to the groupoid of SOEF's on manifolds diffeomorphic to M. The inverse problem is then precisely that of characterizing the image of $\mathcal{F}$ and the problem of alternative Lagrangians is essentially that of describing the extent to which $\mathcal{F}$ fails to be injective.

Concerning the problem of alternative Lagrangians, it is well known that there are several rather trivial ways in which a given regular Lagrangian may be modified and yet still yield the same Euler–Lagrange vector field. Specifically, let L be such a regular Lagrangian; then the Lagrangian $\bar{L}$, where

$$\bar{L} = \lambda L + \tilde{\alpha} + c, \tag{3.4}$$

$\lambda, c \in \mathbf{R}$, and α is a closed one-form on M ($\tilde{\alpha}$ denoting the corresponding real-valued function on TM which is linear in u) does indeed determine the same Euler–Lagrange vector field as L. The term $\tilde{\alpha}$ is known usually as a "gauge term" and is the global, autonomous version of the addition of a total time derivative of a function on M to the Lagrangian. Two Lagrangians L and $\bar{L}$ related as in (3.4) will be called trivially equivalent; the problem of alternative Lagrangians is to be solved modulo this equivalence relation.

An important and basic question relating to the inverse problem is whether the property of a SOEF being a Euler–Lagrange field is invariant under transformations of the form $T\phi$, for ϕ a diffeomorphism of M. This fundamental, conceptual point is usually not addressed in the literature, though the answer to the question just posed can hardly be said to be obvious, given the definitions of a SOEF and the Euler–Lagrange field. In fact, let us apply the diffeomorphism $T\phi$ to either side of (3.3), noting that since Δ and S are

natural objects on TM they are certainly preserved by $T\phi$, that is, $\Delta \cdot T\phi = \Delta$ and $S \cdot T\phi = S$; one obtains

$$i((T\phi)_*^{-1}\Lambda)\omega_{L\cdot T\phi} = -d(\Delta(L\cdot T\phi) - L\cdot T\phi). \quad (3.5)$$

Equation (3.5) says precisely that $(T\phi)_*^{-1}\Lambda$ is the Euler–Lagrange vector field corresponding to the regular Lagrangian $L\cdot T\phi$.

In terms of an adapted coordinate system (x^i, u^i) on TM, the f^j's in a Euler–Lagrange field [see (2.3)] are determined in terms of the Lagrangian L according to the conditions

$$\frac{\partial^2 L}{\partial u^i \partial u^j} f^j = \frac{\partial L}{\partial x^i} - u^j \frac{\partial^2 L}{\partial x^j \partial u^i}. \quad (3.6)$$

The reader may care to give a proof in local coordinates of the result derived in the previous paragraph using (3.6). [One has to check that the f^j's defined by (3.6) transform according to (2.10).] Perhaps the most obvious and direct approach to the inverse problem is to consider (3.6) as a system of m second-order partial differential equations for the unknown L; one has to give necessary and sufficient conditions on the f^j's for there to exist a solution L which also satisfies the transversality condition (3.2). Of course this is a highly nontrivial problem. Now an answer of sorts to the inverse problem, as is well known, is provided by the Helmholtz conditions.[1,2] However, this "solution" is no more an answer than that which says that a Lagrangian exists, if and only if there is a regular solution to (3.6). Indeed, the Helmholtz conditions, as given by Crampin[1] for example, are really only a way of recasting (3.6) as a first-order system of differential equations in terms of the intermediate variables $g_{ij} = \partial^2 L / \partial u^i \partial u^j$ (together with some purely algebraic conditions on the g_{ij}'s).

The one case in which (3.6) can be analyzed completely is when $m = 1$ so that (3.6) reduces to a single equation. In that case the existence of a Lagrangian L follows, at least if one assumes that the single function f is analytic in x and u, from the Cauchy–Kowalewski theorem. Furthermore, L can be found such that $\partial L^2/\partial u^2 \neq 0$, at least on an open set in TM, and so L is a regular Lagrangian. As to the problem of alternative Lagrangians, it is easy to verify the following: if L is a regular solution of (3.6) (with $m = 1$), and the energy H_L is defined by $H_L = u(\partial L/\partial u) - L$, then up to trivially equivalent Lagrangians, every other Lagrangian is given by $\bar{L}$ where F is an arbitrary smooth function of H_L and

$$\bar{L} = u \int \frac{F(H_L)du}{u^2}. \quad (3.7)$$

[Of course in (3.7) an arbitrary function of x enters because of the integration with respect to u, but this simply results in the addition of a gauge term to the Lagrangian.]

The case of $m = 1$ is of fairly limited interest in its own right of course; however, it is useful for checking that results conjectured for arbitrary values of m reduce to a correct result for $m = 1$. Furthermore, if one is given a Lagrangian system with m arbitrary, one may always take the "direct product" (in the obvious informal sense) of it with a one-dimensional Lagrangian and the resulting Lagrangian system will be one which admits alternative Lagrangians. Any attempt to solve the problem of alternative Lagrangians then, has to incorporate some way of detecting when this situation occurs; indeed it begs the question of whether alternative Lagrangians always arise in this way.

IV. LAGRANGIANS ANALYTIC IN u

The notion of equivalence of SOEF's introduced in Sec. II, namely, an equivalence that preserves the structure of tangent bundles, suggests that we consider systems of second-order equations like (2.3) in which the f^k's are analytic functions of u. For a diffeomorphism of two tangent bundles which is lifted (or "prolonged") from a diffeomorphism of the corresponding manifolds, preserves all such notions as (real-valued) functions being "polynomial or analytic in the fiber." (On the other hand, it has to be admitted that this assumption of analyticity is a significant restriction; it would exclude, for example, the interesting families of alternative Lagrangians for a particle moving under a spherically symmetric potential given by Henneaux and Shepley[11]).

In this section I investigate what the implications are of expanding the f^j's in powers of u and using the decomposition given by (2.11). I shall begin by deriving some simple consequences of (3.6) in the shape of the following proposition.

Proposition 4.1: Let Γ be an SOEF on M. Then if there exists a Lagrange function L on TM such that Γ is the Euler–Lagrangian vector field of L and if L is analytic in u (about the zero section of TM), Γ is analytic in u. Furthermore, if L and the f^j's are polynomial [in u and u^i, respectively, where (x^i, u^i) is an adapted coordinate system], then the f^j's are at most quadratic polynomials. Finally, if it is assumed simply that L is quadratic in u (and regular), the f^j's are necessarily at most quadratic in u^i.

Proof: The proof of the first statement is quite straightforward. [One may show that the matrix $(\partial^2 L/\partial u^i \partial u^j)^{-1}$ consists of functions analytic in u, the coefficients of which are determined in terms of the coefficients in the series expansion of L; I shall return to this point below.]

The proof of the second statement is clear from (3.6), because if L is of degree, say n, in u, the right-hand side of (3.6) is of degree at most n. Thus the left-hand side is of degree no more than n, which evidently means that the f^j's can be at most quadratic.

To prove the third assertion, differentiate (3.6) fiberwise three times assuming that L is quadratic in u. One easily obtains

$$\frac{\partial^2 L}{\partial u^i \partial u^j} \frac{\partial^3 f^j}{\partial u^k \partial u^m \partial u^n} = 0. \quad (4.1)$$

Now (4.1) implies that the f^j's are quadratic in u^i because the matrix $\partial^2 L/\partial u^i \partial u^j$ is nonsingular.

It is important to appreciate that the converse of each assertion made in Proposition 4.1 is false. Counterexamples can be obtained by considering a free particle (when the f^j's are identically 0) in one dimension and noting some of the remarks made in Sec. III on one-dimensional systems. Similarly it is easy to generalize to appropriate counterexamples with an arbitrary number of dependent variables.

To return to the proof of the first assertion in Proposition 4.1, let us suppose that L is developed as a power series in u. Specifically, let (x^i, u^i) be an adapted coordinate system and suppose

$$L = A + A_i u^i + (1/2!)A_{ij}u^i u^j + (1/3!)A_{ijk}u^i u^j u^k + (1/4!)A_{ijkl}u^i u^j u^k u^l + \cdots, \tag{4.2}$$

where $A, A_i, A_{ij}, A_{ijk}, A_{ijkl}$, etc., are functions of x^i only. Then one may show from (3.6) that the first three terms in f^j are given explicitly by

$$f^j = \frac{\partial A}{\partial x^a}(A^{-1})^{aj} + \left[\left(\frac{\partial A_k}{\partial x^a} - \frac{\partial A_a}{\partial x^k}\right)(A^{-1})^{aj} - \frac{\partial A}{\partial x^a}A_{ikl}(A^{-1})^{ij}(A^{-1})^{al}\right]u^k$$
$$+ \frac{1}{2}\left[-(A^{-1})^{aj}\left(\frac{\partial A_{la}}{\partial x^k} + \frac{\partial A_{ka}}{\partial x^l} - \frac{\partial A_{kl}}{\partial x^a}\right) + \left(\left(\frac{\partial A_a}{\partial x^l} - \frac{\partial A_l}{\partial x^a}\right)A_{ikm} + \left(\frac{\partial A_a}{\partial x^k} - \frac{\partial A_k}{\partial x^a}\right)A_{ilm}\right)(A^{-1})^{ij}(A^{-1})^{am}\right.$$
$$\left. + \frac{\partial A}{\partial x^a}\left((A_{ikm}A_{lnp} + A_{ilm}A_{knp})(A^{-1})^{ij}(A^{-1})^{mp}(A^{-1})^{an} - A_{iklm}(A^{-1})^{am}(A^{-1})^{ij}\right)\right]u^k u^l + \cdots. \tag{4.3}$$

The terms in f_j of degree 3 and higher can be determined, in principle, in a similar manner, the term of degree n depending on the coefficients corresponding to terms in L of degree up to and including $n+2$.

There are some other points worth noting about (4.3). First, if in (4.2) A is constant and the term $A_i u^i$ corresponds to a closed one-form on M, that is, is a pure gauge term, the zeroth- and first-order terms in the expansion (4.3) are 0. Conversely, suppose that one is given a SOEF and that in the expansion of the corresponding f^j's, the zeroth- and first-order terms are 0; then if there is a regular Lagrangian L such that Γ is its Euler-Lagrange vector field, in the expansion (4.2), A must be constant and $A_i u^i$ must be a gauge term. In other words, in looking for such a Lagrangian, one may assume without loss of generality that its lowest-order terms are quadratic in u.

The second point about (4.3) concerns the spray associated to SOEF Γ which is the Euler–Lagrange vector field of a regular Lagrangian L. Suppose that in an adapted coordinate system (x^i, u^i) the Christoffel symbols of this spray are Γ^j_{kl} so that (4.3) gives

$$\Gamma^j_{kl} = -\frac{1}{2}\left[(A^{-1})^{aj}(A_{la,k} + A_{ka,l} - A_{kl,a}) + ((A_{l,a} - A_{a,l})A_{ikm} + (A_{k,a} - A_{a,k})A_{ilm})(A^{-1})^{ij}(A^{-1})^{am}\right.$$
$$\left. + \frac{\partial A}{\partial x^a}\left((A_{ikm}A_{lnp} + A_{ilm}A_{knp})(A^{-1})^{ij}(A^{-1})^{mp}(A^{-1})^{an} - A_{iklm}(A^{-1})^{am}(A^{-1})^{ij}\right)\right]. \tag{4.4}$$

Thus if we interpret A_{ij} as a Riemannian or pseudo-Riemannian metric on M (A_{ij} must be nonsingular if L is to be regular on the zero section of TM), we see that the spray associated to Γ is the Levi connection of A_{ij} if either L is quadratic in u or is trivially equivalent to a Lagrangian whose lowest-order terms are quadratic (and possibly in other cases, too). By performing maniupulations similar to these in Riemannian geometry,[6] one can derive from (4.4)

$$A_{bk,l} = A_{bj}\Gamma^j_{kl} + A_{kj}\Gamma^j_{lb} + B_{bkl}, \tag{4.5}$$

where

$$B_{bkl} = \tfrac{1}{2}[(A_{a,k} - A_{k,a})A_{blm} + 2(A_{a,l} - A_{l,a})A_{bkm} + (A_{a,b} - A_{b,a})A_{klm}](A^{-1})^{am}$$
$$+ \tfrac{1}{2}A_{,a}(A_{blm}A_{knp} + 2A_{bkm}A_{lnp} + A_{klm}A_{bnp})(A^{-1})^{mp}(A^{-1})^{an} - A_{,a}A_{bklm}(A^{-1})^{am}. \tag{4.6}$$

Equation (4.5) can also be written in the form

$$A_{bk;l} = B_{bkl}, \tag{4.7}$$

where the semicolon denotes the covariant derivative with respect to the connection whose components are Γ^j_{kl}. Differentiating (4.7) covariantly again and invoking Ricci's identities which measure the extent to which iterated covariant derivatives fail to commute,[6] one obtains the following integrability conditions:

$$A_{bs}R^s_{rlk} + A_{ks}R^s_{rlb} = B_{bkr;l} - B_{bk;lr}, \tag{4.8}$$

where R^s_{rlk} are the components of the curvature tensor determined by the Γ^j_{kl}'s.

It follows amongst other things from (4.8) that if the right-hand side is 0 (again if L is quadratic or its lowest-order terms are quadratic, for example), that the curvature of the connection associated to Γ has a Ricci tensor which is symmetric.

V. THE INVERSE PROBLEM FOR SPRAYS

I shall consider in this section what is in effect a special case of the inverse problem, but one which is of considerable interest in its own right, namely, when the given SOEF is a spray. We have already seen in Sec. II, that the f^j's being (not necessarily homogeneous) quadratic is an invariant condition, whereas the f^j's being independent of u^i, for example, is not. The special status of quadratic systems is further reinforced in Lagrangian theory by Proposition 4.1. The reason for considering sprays first, as opposed to more general quadratic systems, is that sprays are the most natural kinds of SOEF's from the geometric standpoint. In particular, given a spray on M, one may ask if it is the geodesic flow of the Levi-Civita connection of some Riemannian or pseudo-Riemannian metric on M. This is indeed a special case of the inverse problem because one is asking for a quadratic

Lagrangian for which Λ is the associated Euler–Lagrange vector field.

Suppose then that Λ is a spray corresponding to the second-order system

$$\ddot{x}^j = -\Gamma^j_{ab}\dot{x}^a\dot{x}^b. \tag{5.1}$$

If we look for a Lagrangian analytic in u, by a previous remark we may assume that $A = 0$ and $A_i = 0$ in (4.2). Inserting the remaining terms in (4.2) into (3.6) with the f^j's given by the right-hand side of (5.1), one finds the following conditions for $n = 2,3,\ldots$:

$$nA_{k(i_1\cdots i_{n-1},i_n)} - A_{i_1\cdots i_n,k} = n(n-1)\Gamma^j_{(i_1i_2}A_{i_3\cdots i_n)jk}. \tag{5.2}$$

Thus, for a spray and indeed essentially in that case alone, (3.6) decouples by degree. In other words, (5.2) are precisely the conditions that there should exist a Lagrangian, which is a homogeneous polynomial of degree n in u ($n\geqslant 2$), and, for different values of n, these conditions are independent of each other.

From (5.2) it follows by symmetrization that

$$(n-1)A_{(i_1\cdots i_n,k)} = n(n-1)\Gamma^j_{(i_1i_2}A_{i_3\cdots i_n)k)j}, \tag{5.3}$$

which in turn, by choosing k as a distinguished index in the symmetrization in the left-hand side of (5.3), implies that

$$[1/(n+1)]A_{i_1\cdots i_n,k} + [n/(n+1)]A_{k(i_1\cdots i_{n-1},i_n)} = n\Gamma^j_{(i_1i_2}A_{i_3\cdots i_n)k)j}. \tag{5.4}$$

From (5.2) and (5.4) we easily obtain

$$A_{i_1\cdots i_n,k} = \binom{n+1}{2}\Gamma^j_{(i_1i_2}A_{i_3\cdots i_n)kj} - \binom{n}{2}\Gamma^j_{(i_1i_2}A_{i_3\cdots i_n)kj}. \tag{5.5}$$

Equation (5.5) can be rewritten as

$$A_{i_1\cdots i_n,k} = \Gamma^j_{i_1k}A_{ji_2\cdots i_n} + \Gamma^j_{i_2k}A_{i_1ji_3\cdots i_n} + \cdots + \Gamma^j_{i_nk}A_{i_1\cdots i_{n-1}j}, \tag{5.6}$$

which in turn is equivalent to

$$A_{i_1\cdots i_n;k} = 0, \tag{5.7}$$

where the semicolon denotes the covariant derivative with respect to the connection defined by the Γ^i_{jk}'s. Conversely, since (5.7) is equivalent to (5.5) and also implies (5.3), it is clear that (5.7) is equivalent to (5.2). I summarize the preceding discussion in the following theorem.

Theorem 5.1: Given a spray Λ on M, a function $\overline{L}$ on TM analytic in u is a regular Lagrangian for Λ iff $\overline{L}$ satisfies the following conditions: $\overline{L}$ is trivially equivalent to a Lagrangian L which has an expansion of the form (4.2) in which $A = 0$ and $A_i = 0$, A_{ij} is nonsingular and each nonzero term in (4.2) corresponds to a symmetric, covariant tensor field on M parallel with respect to the parallel transport defined by the connection associated to Λ.

A number of observations about Theorem 5.1 are in order. First of all, given a spray Λ, if there is to be a regular Lagrangian whose Euler–Lagrange field is Λ, (5.7) must be satisfied for some nonsingular A_{ij} in the case $n = 2$. In other words, Λ must be the geodesic spray of the metric A_{ij}. Suppose that such a metric A_{ij} exists; then $L = \frac{1}{2}A_{ij}u^iu^j$ is a regular Lagrangian for Λ and we may enquire whether an alternative Lagrangian exists. In fact, such a Lagrangian will exist if either one can find another metric compatible with the connection defined by Λ or else there is symmetric tensor $A_{i_1\cdots i_n}$ of valence n parallel with respect to parallel transport defined by that connection. Condition (5.7) is very restrictive; despite this, when a metric A_{ij} exists, all tensor powers of A_{ij} satisfy (5.7). Thus $A_{(ij}A_{kl)}$ satisfies (5.7) with $n = 4$ because

$$\begin{aligned}[A_{(ij}A_{kl)}]_{;m} &= A_{(ij}[A_{kl);m}] + A_{(kl}[A_{ij);m}]\\ &= 2A_{(ij}A_{kl);m}\\ &= 0,\end{aligned}$$

since $A_{kl;m} = 0$. So for a spray Λ compatible with a metric A_{ij}, there are always many (nontrivial) alternative Lagrangians obtained by adding to the Lagrangian L functions on TM corresponding to symmetric tensor powers of the metric.

Another somewhat different way in which solutions to (5.7) arise is in the context of locally symmetric spaces.[7] A manifold M with a metric A_{ij} is said to be locally symmetric if the curvature tensor R^i_{jkl} is parallel with respect to the parallel transport of the Levi-Civita connection defined by A_{ij}, in other words, if

$$R^i_{jkl;m} = 0. \tag{5.8}$$

Equation (5.8) implies of course that

$$R^j_{jkl;m} = 0, \tag{5.9}$$

that is, the Ricci tensor $R_{kl} = R^j_{jkl}$ is parallel. Since we are dealing with a manifold with a metric, the Ricci tensor is also symmetric and thus satisfies (5.7) with $n = 2$. Of course it may be that R_{kl} is a constant multiple of A_{ij} in which case (M,A_{ij}) is said to be an Einstein manifold. Furthermore, there is no reason to suppose in general that R_{ij} is nondegenerate and so may not serve as an alternative metric compatible with the connection ∇.

Again suppose that Λ is a spray on M which is given in an adapted coordinate system (x^i, u^i) by

$$\Lambda = u^i\frac{\partial}{\partial x^i} - \Gamma^i_{jk}u^ju^k\frac{\partial}{\partial u^i}. \tag{5.10}$$

Then one may readily show that the necessary and sufficient condition that a polynomial homogeneous of degree n in u, $B_{i_1\cdots i_n}u^{i_1}\cdots u^{i_n}$ say, is a first integral of Λ is

$$B_{(i_1\cdots i_n;i_{n+1})} = 0. \tag{5.11}$$

A symmetric, covariant tensor field $B_{i_1\cdots i_n}$ which satisfies (5.11) is said to be a Killing tensor field of the connection ∇ corresponding to Λ.[12,13] [The notion of a contravariant Killing vector on a manifold with metric is extremely well known. The Killing condition on the corresponding covariant object is precisely (5.11) with $n = 1$, so that (5.11) is the natural generalization of this condition.] Equation (5.11) is of course a weaker condition than (5.7). In particular, when looking for Lagrangians L corresponding to Λ, each term in the expansion (4.2) of degree 2 or more is a first integral of Λ. This shows how restrictive (5.7) is: to the

knowledge of the author, there are no known examples of manifolds with a metric that have a homogeneous first integral of degree n in u, which is notrivial when $n>2$. [A Killing tensor of degree n is said to be trivial if it consists of a (finite) sum of symmetrized products of lower-order Killing tensors.] For $n=2$, however, a limited number of examples are known such as the Kerr metric[12] and the Ricci tensor in locally symmetric spaces as described above.

The conditions given in Theorem 5.1 for a spray to admit a Lagrangian are easily extended to systems in which the f^j's are quadratic in u^i, though the geometric interpretation becomes somewhat more contrived. Indeed, instead of (5.1) consider the following system:

$$\ddot{x}^j = -(\Gamma^j + \Gamma^j_a u^a + \Gamma^j_{ab} u^a u^b), \tag{5.12}$$

where Γ^j, Γ^j_a, and Γ^j_{ab} are functions of x^i only. Then if one seeks a Lagrangian of the form (4.2), one finds by modifying (5.2)–(5.7) that the following conditions are necessary and sufficient for the existence of such a Lagrangian:

$$A_{,i} = -A_{ij}\Gamma^j, \tag{5.13}$$

$$A_{k,i} - A_{i,k} = -A_{ij}\Gamma^j_k, \tag{5.14}$$

$$A_{i_1\cdots i_{n,k}} = \frac{1}{n-1}\Gamma^j A_{jki_1\cdots i_n} + \frac{n(n+1)}{2(n-1)}\Gamma^j_{(i_1}A_{i_2\cdots i_n k)j} - (n/2)\Gamma^j_{(i_1}A_{i_2\cdots i_n)kj} \quad (n\geqslant 2). \tag{5.15}$$

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The inverse scattering problem for the soft ellipsoid

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A soft triaxial ellipsoid, of unknown semiaxes and orientation, is excited into secondary radiation by a plane acoustic wave of a fixed low frequency. It is proved that one measurement of the leading low-frequency coefficient and exactly six measurements of the second low-frequency coefficient of the real part of the forward or the backward scattering amplitude are enough to specify completely both the semiaxes, as well as the orientation of the ellipsoid. Therefore, only the first two low-frequency coefficients of the real part of the scattering amplitude are needed in order to solve the inverse scattering problem for the soft ellipsoid. For the case of spheroids, the number of measurements is restricted to one for the first and three for the second coefficient. Finally, the sphere is specified by a single measurement of the leading coefficient. The special cases where the orientation or the semiaxes are known are also discussed.

I. INTRODUCTION

The problem of scattering of a plane acoustic wave of fixed frequency by a soft body has a history of approximately one century. Its complete mathematical analysis can be found in Ref. 1, where also the low-frequency approximation of the wave problem has been reduced to certain potential problems through Neumann series expansions. Sleeman[2] has applied Kleinman's method[1] to the case of an ellipsoid and he evaluated the low-frequency coefficients up to the second order in terms of elliptic functions. In Ref. 3, a different technique has been used to evaluate the four leading coefficients of the scattering amplitude, using also Lamé products but in their algebraic form, which simplifies the final results considerably. In fact, the scattering amplitude is given explicitly in Ref. 3, in terms of the three semiaxes of the ellipsoid, the directional cosines of incidence, the directional cosines of observation, and four well known elliptic integrals connected through two algebraic relations. The actual geometry of the scatterer is implicit in the values of these elliptic integrals, while the directions of incidence and orientation, which are at our disposal to control, specify the relative orientation of the ellipsoid. It is in fact the simplicity of the expression of the fourth low-frequency coefficient of the scattering amplitude that allows for an exact solution of the corresponding inverse problem.

In order to solve completely the inverse problem, all we need to specify are the three semiaxes as well as the three Euler angles that fix the position of the principal axes of the ellipsoid. Therefore, we need to excite ("see") the ellipsoid from six different angles and for each one of them to measure the forward or the backward scattering amplitude, which conveys all the information about the scatterer that can be "seen" from the particular direction of incidence. It turns out that these six measurements give rise to a highly nonlinear system involving four elliptic integrals. Therefore, we need one more piece of information to effectively solve the inverse problem. The choice of the six directions of incidence should be such as to make an optimum use of the symmetry inherited in the ellipsoid. We note that our technique depends crucially upon the inversion symmetry, as well as on the particular form that the scattering theorem assumes for scatterers having inversion symmetry.[4]

We remark that as long as we are in the low-frequency realm no measurement of any frequency is necessary.[5] Also, only the expression of the zeroth- and fourth-order low-frequency coefficients of the normalized scattering amplitude,[3] or equivalently, the first two nonvanishing terms of its real part are needed for the complete solution of the inverse problem.

As it is well known,[5] the inverse scattering problem is intrinsically nonlinear. In the case of the ellipsoid the nonlinearities enter the problem via the elliptic integrals, the second and fourth powers of the values of the semiaxes, and the quadratic expressions of the components of the directions of incidence and observation. To a large extent, the worst part of these nonlinearities has been eliminated by algebraic manipulations and the use of the seventh measurement. Nevertheless we cannot avoid dealing at least with one standard elliptic integral for the determination of the semiaxes. The effect of nonlinearity in finding the orientation is reflected upon the nonlinear expressions providing the three Euler angles.

Angell and Kleinman have reduced the inverse scattering problem for an ellipsoid to a constrained optimization problem.[6] They have considered all the physically important boundary conditions in acoustics as well as in electromagnetism except the scalar Dirichlet problem explored in the present paper by a completely different method.

After giving all the necessary information from the solution of the direct problem in Sec. II, we proceed to Sec. III where the solution of the inverse scattering problem is given in its generality. The special cases of known orientation of geometries with higher symmetry are discussed in Sec. IV.

II. THE DIRECT PROBLEM

Let S be the ellipsoid

$$x_1^2/a_1^2 + x_2^2/a_2^2 + x_3^2/a_3^2 = 1\,, \tag{1}$$

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where $0<a_3<a_2<a_1<+\infty$ are the three semiaxes and $\hat{\mathbf{x}}_1$, $\hat{\mathbf{x}}_2$, $\hat{\mathbf{x}}_3$ are denoting the unit vectors of the orthogonal Cartesian system that coincides with the principal axes of the given ellipsoid. Suppressing the harmonic time dependence $\exp\{-i\omega t\}$, the direct scattering problem for (1) consists in finding a solution u of the Helmholtz equation

$$\Delta u + k^2 u = 0, \tag{2}$$

in the region V, exterior to S, which assumes the values

$$u = -e^{i\mathbf{k}\cdot\mathbf{r}}, \tag{3}$$

on S and the asymptotic form

$$r\left(\frac{\partial u}{\partial r} - iku\right) = o(1) \tag{4}$$

as $r\to+\infty$. The vector $\mathbf{k}$ determines the direction of propagation of the incident wave $\exp\{i\mathbf{k}\cdot\mathbf{r}\}$, while its magnitude k is the wave number. Far away from the scatterer, the scattered field u has the asymptotic form

$$u(\mathbf{r}) = g(\hat{\mathbf{r}},\hat{\mathbf{k}})h(kr) + O(1/r^2), \tag{5}$$

where $h(x) = e^{ix}/ix$ and $g(\hat{\mathbf{r}},\hat{\mathbf{k}})$ is the normalized (dimensionless) scattering amplitude which describes the response of the scatterer in the direction $\hat{\mathbf{r}}$ to plane wave excitation of direction $\hat{\mathbf{k}}$. Due to the symmetry of the ellipsoid the scattering amplitude satisfies the following relations[4]:

$$g(\hat{\mathbf{r}},\hat{\mathbf{k}}) = g(\hat{\mathbf{k}},\hat{\mathbf{r}}) \tag{6}$$

and

$$-\operatorname{Re} g(\hat{\mathbf{k}},\hat{\mathbf{k}}) = \frac{1}{4\pi}\int_{|\hat{\mathbf{p}}|=1} |g(\hat{\mathbf{p}},\hat{\mathbf{k}})|^2\, d\Omega(\hat{\mathbf{p}}). \tag{7}$$

As a consequence of (6) and (7) if the amplitude g has the low-frequency expansion[3]

$$g(\hat{\mathbf{r}},\hat{\mathbf{k}}) = ikA_1(\hat{\mathbf{r}},\hat{\mathbf{k}}) + k^2A_2(\hat{\mathbf{r}},\hat{\mathbf{k}}) + ik^3A_3(\hat{\mathbf{r}},\hat{\mathbf{k}}) + k^4A_4(\hat{\mathbf{r}},\hat{\mathbf{k}}) + O(k^5) \tag{8}$$

as $k\to 0+$, and if the leading two coefficients of the $\operatorname{Im} g(\hat{\mathbf{r}},\hat{\mathbf{k}})$ are known, then the leading two coefficients of $\operatorname{Re} g(\hat{\mathbf{r}},\hat{\mathbf{k}})$ can be found from[7]

$$A_2(\hat{\mathbf{r}},\hat{\mathbf{k}}) = -\frac{1}{4\pi}\int_{|\hat{\mathbf{p}}|=1} A_1(\hat{\mathbf{p}},\hat{\mathbf{r}})A_1(\hat{\mathbf{p}},\hat{\mathbf{r}})d\Omega(\hat{\mathbf{p}}) \tag{9}$$

and

$$A_4(\hat{\mathbf{r}},\hat{\mathbf{k}}) = -\frac{1}{4\pi}\int_{|\hat{\mathbf{p}}|=1} [A_1(\hat{\mathbf{p}},\hat{\mathbf{r}})A_3(\hat{\mathbf{p}},\hat{\mathbf{k}}) + A_2(\hat{\mathbf{p}},\hat{\mathbf{r}})A_2(\hat{\mathbf{p}},\hat{\mathbf{k}}) + A_3(\hat{\mathbf{p}},\hat{\mathbf{r}})A_1(\hat{\mathbf{p}},\hat{\mathbf{k}})]d\Omega(\hat{\mathbf{p}}). \tag{10}$$

The actual coefficients of $g(\hat{\mathbf{r}},\hat{\mathbf{k}})$ for the case of the soft ellipsoid are given by[3]

$$A_1(\hat{\mathbf{r}},\hat{\mathbf{k}}) = -1/I, \tag{11}$$

$$A_2(\hat{\mathbf{r}},\hat{\mathbf{k}}) = -1/I^2, \tag{12}$$

$$A_3(\hat{\mathbf{r}},\hat{\mathbf{k}}) = 1/I^3 - (1/3I)(a_1^2+a_2^2+a_3^2) + (1/3I^2)(a_1^4I_1 + a_2^4I_2 + a_3^4I_3) - \frac{1}{3}\left(\frac{i_1o_1}{I_1} + \frac{i_2o_2}{I_2} + \frac{i_3o_3}{I_3}\right) + (1/6I)(i_1^2a_1^2 + i_2^2a_2^2 + i_3^2a_3^2) + (1/6I)(o_1^2a_1^2 + o_2^2a_2^2 + o_3^2a_3^2), \tag{13}$$

$$A_4(\hat{\mathbf{r}},\hat{\mathbf{k}}) = 1/I^4 - (5/9I^2)(a_1^2+a_2^2+a_3^2) + (2/3I^3)(a_1^4I_1 + a_2^4I_2 + a_3^4I_3) + (1/6I^2)(i_1^2a_1^2 + i_2^2a_2^2 + i_3^2a_3^2) + (1/6I^2)(o_1^2a_1^2 + o_2^2a_2^2 + o_3^2a_3^2), \tag{14}$$

where $\hat{\mathbf{k}} = (i_1,i_2,i_3)$, $\hat{\mathbf{r}} = (o_1,o_2,o_3)$,

$$I = \frac{1}{2}\int_0^{+\infty} \frac{dx}{\sqrt{x+a_1^2}\sqrt{x+a_2^2}\sqrt{x+a_3^2}}, \tag{15}$$

$$I_n = \frac{1}{2}\int_0^{+\infty} \frac{dx}{(x+a_n^2)\sqrt{x+a_1^2}\sqrt{x+a_2^2}\sqrt{x+a_3^2}}, \quad n=1,2,3. \tag{16}$$

The four elliptic integrals I, I_1, I_2, I_3 are related via the formulas

$$a_1a_2a_3(I_1+I_2+I_3) = 1, \qquad a_1^2I_1 + a_2^2I_2 + a_3^2I_3 = I. \tag{17}$$

In particular,

$$-\operatorname{Re} g(\hat{\mathbf{k}},\hat{\mathbf{k}}) = k^2/I^2 + k^4[T - (1/3I^2)(i_1^2a_1^2 + i_2^2a_2^2 + i_3^2a_3^2)] + O(k^6), \quad k\to 0+, \tag{18}$$

where

$$T = -1/I^4 + (5/9I^2)(a_1^2+a_2^2+a_3^2) - (2/3I^3)(a_1^4I_1 + a_2^4I_2 + a_3^4I_3). \tag{19}$$

The parameter T depends only on the semiaxes of the ellipsoid and it is independent of its orientation. The reason why we choose to work with the real, instead of the imaginary, part of g is due to the fact that the coefficient A_4 has only one nonisotropic term connecting the directional cosines of $\hat{\mathbf{k}}$ to the corresponding semiaxes, while the coefficient A_3 involves two such terms connecting $\hat{\mathbf{k}}$ to the elliptic integrals I_n, $n=1,2,3$. Then the only really "bad" part in A_4 is the expression T which is evaluated by introducing one more measurement.

Furthermore, expression (14) and hence also (18) provide the same value independently on whether one measures the forward or the backward scattering amplitude.

III. THE INVERSE PROBLEM

The question we try to answer in this section is the following. Suppose we have a way to measure the coefficients $A_2(\hat{\mathbf{k}},\hat{\mathbf{k}})$ and $A_4(\hat{\mathbf{k}},\hat{\mathbf{k}})$ of $g(\hat{\mathbf{k}},\hat{\mathbf{k}})$, how many measurements (corresponding to different $\hat{\mathbf{k}}$'s) are needed in order to effectively specify the ellipsoid (1) as well as its orientation?

As is shown in the sequel we need to know A_2 for a fixed $\hat{\mathbf{k}}$ and A_4 for six different directions of $\hat{\mathbf{k}}$.

In fact, let

$$m_0 = -A_2(\hat{\mathbf{k}},\hat{\mathbf{k}}) \tag{20}$$

and

$$m_j = -A_4(\hat{\mathbf{k}}_j,\hat{\mathbf{k}}_j), \quad j=1,2,3,4,5,6, \tag{21}$$

be the values obtained by the corresponding measurements.

Let $\hat{\mathbf{k}}'$ be an arbitrary direction,

$$\hat{\mathbf{k}}'_j = \hat{\mathbf{x}}'_j, \quad j = 1,2,3, \tag{22}$$

and

$$\begin{aligned} \hat{\mathbf{k}}'_4 &= (1/\sqrt{2})(\hat{\mathbf{x}}'_1 + \hat{\mathbf{x}}'_2) \\ \hat{\mathbf{k}}'_5 &= (1/\sqrt{2})(\hat{\mathbf{x}}'_2 + \hat{\mathbf{x}}'_3), \\ \hat{\mathbf{k}}'_6 &= (1/\sqrt{2})(\hat{\mathbf{x}}'_3 + \hat{\mathbf{x}}'_1), \end{aligned} \tag{23}$$

where $\{\hat{\mathbf{x}}'_1, \hat{\mathbf{x}}'_2, \hat{\mathbf{x}}'_3\}$ form an orthonormal base of an arbitrary chosen Cartesian system whose origin coincides with the centroid of the ellipsoid.

Let $\mathbf{P}$ be the orthogonal matrix that transforms (by rotation) the arbitrarily chosen primed system x'_1, x'_2, x'_3 to the unprimed system x_1, x_2, x_3 determined by the principal directions of the ellipsoid, i.e.,

$$\mathbf{r} = \mathbf{P}\mathbf{r}'. \tag{24}$$

Of course, the matrix $\mathbf{P}$ is not known, since the orientation of the ellipsoid is not known, but its existence and its uniqueness within the orthogonal group is ensured by the orthogonality of both the chosen unprimed system and the system of principal axes of the ellipsoid. The knowledge of the matrix $\mathbf{P}$ will provide the exact orientation of the ellipsoid. The elements P_{ij} of $\mathbf{P}$ are expressed via the three Euler angles φ, θ, y (Ref. 8) as follows:

$$\begin{aligned} P_{11} &= \cos\varphi \cos y - \cos\theta \sin\varphi \sin y, \\ P_{12} &= \sin\varphi \cos y + \cos\theta \cos\varphi \sin y, \\ P_{13} &= \sin\theta \sin y; \end{aligned} \tag{25}$$

$$\begin{aligned} P_{21} &= -\cos\varphi \sin y - \cos\theta \sin\varphi \cos y, \\ P_{22} &= -\sin\varphi \sin y + \cos\theta \cos\varphi \cos y, \\ P_{23} &= \sin\theta \cos y; \end{aligned} \tag{26}$$

$$\begin{aligned} P_{31} &= \sin\theta \sin\varphi, \\ P_{32} &= -\sin\theta \cos\varphi, \\ P_{33} &= \cos\theta. \end{aligned} \tag{27}$$

Therefore, the orientation of the ellipsoid is known whenever the three Euler angles, φ, θ, y are known.

Since the form (18) for the scattering amplitude is referred to as the principal axes system it follows that (18) holds true after the transformation $\mathbf{P}$ has been applied to the directions of incidence $\hat{\mathbf{k}}$, i.e.,

$$\hat{\mathbf{k}}_j = \mathbf{P}\hat{\mathbf{k}}'_j, \quad j = 1,2,3,4,5,6. \tag{28}$$

Consequently,

$$m_0 = 1/I^2 \tag{29}$$

and

$$m_j = T - (1/3I^2)(\hat{\mathbf{k}}_j)^t \mathbf{A}\hat{\mathbf{k}}_j \tag{30}$$

for $j = 1,2,...,6$, where

$$\mathbf{A} = \begin{bmatrix} a_1^2 & 0 & 0 \\ 0 & a_2^2 & 0 \\ 0 & 0 & a_3^2 \end{bmatrix}. \tag{31}$$

In view of (28) and (29), Eqs. (30) take the form

$$3(T - m_j)/m_0 = (\hat{\mathbf{k}}'_j)^t \mathbf{P}^t \mathbf{A} \mathbf{P} (\hat{\mathbf{k}}'_j), \tag{32}$$

for $j = 1,2,...,6$.

Substituting (22) and (23) into (32) we obtain the following nonlinear system of equations for the unknown quantities $\varphi, \theta, y, a_1, a_2, a_3$:

$$P_{11}^2 a_1^2 + P_{21}^2 a_2^2 + P_{31}^2 a_3^2 = 3(T - m_1)/m_0, \tag{33}$$

$$P_{12}^2 a_1^2 + P_{22}^2 a_2^2 + P_{32}^2 a_3^2 = 3(T - m_2)/m_0, \tag{34}$$

$$P_{13}^2 a_1^2 + P_{23}^2 a_2^2 + P_{33}^2 a_3^2 = 3(T - m_3)/m_0, \tag{35}$$

$$(P_{11} + P_{12})^2 a_1^2 + (P_{21} + P_{22})^2 a_2^2 + (P_{31} + P_{32})^2 a_3^2 = 6(T - m_4)/m_0, \tag{36}$$

$$(P_{12} + P_{13})^2 a_1^2 + (P_{22} + P_{23})^2 a_2^2 + (P_{32} + P_{33})^2 a_3^2 = 6(T - m_5)/m_0, \tag{37}$$

$$(P_{11} + P_{13})^2 a_1^2 + (P_{21} + P_{23})^2 a_2^2 + (P_{31} + P_{33})^2 a_3^2 = 6(T - m_6)/m_0. \tag{38}$$

By virtue of (33)–(35), Eqs. (36)–(38) can be written as

$$P_{11}P_{12}a_1^2 + P_{21}P_{22}a_2^2 + P_{31}P_{32}a_3^2 = 3(m_1 + m_2 - 2m_4)/2m_0, \tag{39}$$

$$P_{12}P_{13}a_1^2 + P_{22}P_{23}a_2^2 + P_{32}P_{33}a_3^2 = 3(m_2 + m_3 - 2m_5)/2m_0, \tag{40}$$

$$P_{11}P_{13}a_1^2 + P_{21}P_{23}a_2^2 + P_{31}P_{33}a_3^2 = 3(m_3 + m_1 - 2m_6)/2m_0. \tag{41}$$

Equations (33), (34), (35), (39), (40), and (41) can be combined in the following matrix form:

$$\mathbf{P}^t \mathbf{A} \mathbf{P} = (3T/m_0)\mathbf{I} + \mathbf{M}, \tag{42}$$

where $\mathbf{M}$ is the real symmetric matrix of measurements of the A_4 coefficient given by

$$M = \frac{3}{2m_0} \begin{bmatrix} -2m_1 & m_1 + m_2 - 2m_4 & m_3 + m_1 - 2m_6 \\ m_1 + m_2 - 2m_4 & -2m_2 & m_2 + m_3 - 2m_5 \\ m_3 + m_1 - 2m_6 & m_2 + m_3 - 2m_5 & -2m_3 \end{bmatrix}. \tag{43}$$

The matrix $\mathbf{M}$ has the real eigenvalues $\lambda_1, \lambda_2, \lambda_3$ and its eigenvectors form an orthonormal basis in $\mathbf{R}^3$.

Equation (42) is also written as

$$\mathbf{A} - (3T/m_0)\mathbf{I} = \mathbf{P}\mathbf{M}\mathbf{P}^t. \tag{44}$$

Since the left-hand side of (44) is a diagonal matrix, $\mathbf{M}$ is a real symmetric matrix, and $\mathbf{P}$ is orthogonal, it follows that the eigenvalues of $\mathbf{M}$ are given by

$$\lambda_k = a_k^2 - 3T/m_0, \quad k = 1,2,3, \tag{45}$$

while the columns of $\mathbf{P}^t$ are the corresponding orthonormal eigenvectors. Therefore, the squares of the three semiaxes are given by

$$a_k^2 = \lambda_k + 3T/m_0\,, \quad k = 1,2,3\,. \tag{46}$$

The value of the expression T can be calculated from (29), which in view of (15) is written as

$$\int_0^{+\infty} \frac{dx}{\sqrt{x+\lambda_1+3T/m_0}\sqrt{x+\lambda_2+3T/m_0}\sqrt{x+\lambda_3+3T/m_0}} = \frac{2}{\sqrt{m_0}}\,. \tag{47}$$

The transformation

$$x = (\lambda_1-\lambda_3)/t^2 - (\lambda_1+3T/m_0) \tag{48}$$

brings the elliptic integral in (47) to its canonical form

$$F(\varphi_0,\alpha_0) = \int_0^{\sin\varphi_0} \frac{dt}{\sqrt{1-t^2}\sqrt{1-t^2\sin^2\alpha_0}} = \sqrt{\frac{\lambda_1-\lambda_3}{m_0}}\,, \tag{49}$$

where $F(\varphi_0,\alpha_0)$ denotes the incomplete elliptic integral of the first kind,[9] with amplitude

$$\varphi_0 = \sin^{-1}\sqrt{(\lambda_1-\lambda_3)/(\lambda_1+3T/m_0)} \tag{50}$$

and modular angle

$$\alpha_0 = \sin^{-1}\sqrt{(\lambda_1-\lambda_2)/(\lambda_1-\lambda_3)}\,. \tag{51}$$

From (50) we obtain the value of T as

$$T = [m_0(\lambda_1-\lambda_3)/3]\cot^2\varphi_0 - m_0\lambda_3/3\,. \tag{52}$$

Putting everything together the steps we need to follow in order to evaluate the semiaxes and the orientation of the ellipsoid are the following: (a) we measure, in the forward direction, A_2 for any $\hat{\mathbf{k}}$ and A_4 for the six directions given by (22) and (23); (b) we write down the matrix of measurements $\mathbf{M}$ as it is given by (43); (c) we evaluate the eigenvalues $\lambda_1,\lambda_2,\lambda_3$ (this involves the solution of a cubic equation) and the eigenvectors (P_{11},P_{12},P_{13}), (P_{21},P_{22},P_{23}), and (P_{31},P_{32},P_{33}) of $\mathbf{M}$; and (d) using tables, or a numerical procedure, we evaluate T from (49)–(52). Then, the semiaxes are given by

$$a_1^2 = (\lambda_1-\lambda_3)\cot^2\varphi_0 + (\lambda_1-\lambda_3)\,, \tag{53}$$

$$a_2^2 = (\lambda_1-\lambda_3)\cot^2\varphi_0 + (\lambda_2-\lambda_3)\,, \tag{54}$$

$$a_3^2 = (\lambda_1-\lambda_3)\cot^2\varphi_0\,, \tag{55}$$

while the orientation is given by the Euler angles

$$\varphi = \sin^{-1}(P_{31}/\sqrt{1-P_{33}^2})\,, \tag{56}$$

$$\theta = \sin^{-1}\sqrt{1-P_{33}^2}\,, \tag{57}$$

$$y = \sin^{-1}(P_{13}/\sqrt{1-P_{33}^2})\,, \tag{58}$$

which are derived from (25)–(27).

IV. DEGENERATE CASES

The case of a spheroid corresponds to $a_2 = a_3$, while the rotational symmetry reduces the number of independent parameters for the determination of the orientation to 2. Therefore, we only need to evaluate the two semiaxes a_1, a_2 and the two Euler angles φ, θ that fix the axis of the spheroid. Assuming $y = 0$, the orthogonal transformation that brings the arbitrarily chosen primed system to the system of principal axes of the spheroid, takes the form

$$\mathbf{P}_0 = \begin{bmatrix} \cos\varphi & \sin\varphi & 0 \\ -\cos\theta\sin\varphi & \cos\theta\cos\varphi & \sin\theta \\ \sin\theta\sin\varphi & -\sin\theta\cos\varphi & \cos\theta \end{bmatrix}. \tag{59}$$

Then, the m_1,m_2,m_3 measurements provide us with the system

$$a_1^2\cos^2\varphi + a_2^2\sin^2\varphi = 3(T-m_1)/m_0\,, \tag{60}$$

$$a_1^2\sin^2\varphi + a_2^2\cos^2\varphi = 3(T-m_2)/m_0\,, \tag{61}$$

$$a_2^2 = 3(T-m_3)/m_0\,, \tag{62}$$

which has the solution

$$a_1^2 = 3(T-m_1-m_2+m_3)/m_0\,, \tag{63}$$

$$a_2^2 = 3(T-m_3)/m_0\,, \tag{64}$$

$$\sin^2\varphi = (m_2-m_3)/(m_1+m_2-2m_3)\,. \tag{65}$$

Therefore, the three measurements along the axes are enough to determine both semiaxes as well as the first Euler angle φ. Using (59) into Eqs. (39)–(41) we confirm that the measurements m_4,m_5,m_6 are not independent any more and they can be expressed in terms of m_1, m_2, and m_3.

Note that any rotation around the axis of the spheroid, which is fixed by the angles φ,θ, leaves the spheroid invariant. Therefore, the measurements m_1,m_2,m_3 will be invariant under any rotation by the third Euler angle y. In particular, if $y = \pi/2$, then the elements of the first column of $\mathbf{P}_{\pi/2}$ are given by

$$\begin{aligned} P_{\pi/2,11} &= -\cos\theta\sin\varphi\,, \\ P_{\pi/2,21} &= -\cos\varphi\,, \\ P_{\pi/2,31} &= \sin\theta\sin\varphi\,, \end{aligned} \tag{66}$$

and since the value of m_1 is still the same, Eq. (33) yields

$$a_1^2\cos^2\theta\sin^2\varphi + a_2^2(\cos^2\varphi + \sin^2\theta\sin^2\varphi) = 3(T-m_1)/m_0\,, \tag{67}$$

or, in view of (63) and (64),

$$\cos^2\theta = (m_1-m_3)/(m_2-m_3)\,. \tag{68}$$

The value of T is obtained from (29) where the elliptic integral (15) can be evaluated in this case and its value is given by[3]

$$I = \begin{cases} (1/\sqrt{a_1^2-a_2^2})\cosh^{-1}(a_1/a_2), & a_1 > a_2\,, \\ (1/\sqrt{a_2^2-a_1^2})\cos^{-1}(a_1/a_2), & a_1 < a_2\,. \end{cases} \tag{69}$$

Therefore,

$$T = [(\delta+1)m_3 - m_1 - m_2]/(\delta-1)\,, \tag{70}$$

where

$$\delta = \begin{cases} \cos h^2[\sqrt{3(2m_3 - m_1 - m_2)}/m_0], & a_1 > a_2, \\ \cos^2[\sqrt{3(m_1 + m_2 - 2m_3)}/m_0], & a_1 < a_2. \end{cases} \tag{71}$$

Consequently, rotational symmetry reduces the number of necessary measurements by 3.

The case of radial symmetry reduces the number of measurements by another 3. In fact, for a sphere the only quantity we need to evaluate is its radius a and this comes out from the m_0 measurement, since $I = a^{-1}$ and $a = \sqrt{m_0}$.

Of course, the reduction of the total number of measurements, from seven for the ellipsoid, to four for the spheroids, and to one for the sphere assumes *a priori* information about the actual shape of the scatterer. If there is no such information at our disposal then we have to perform all seven measurements and then decide whether the scatterer is an ellipsoid, a spheroid, or a sphere by looking at the number of equal eigenvalues of the matrix of measurements **M**.

Finally, we discuss the case where the orientation or the semiaxes are known. In particular, if the orientation is known, then by choosing the coordinate system along the principal axes the three Eqs. (33)–(35) take the form

$$a_k^2 = 3(T - m_k)/m_0, \quad k = 1,2,3. \tag{72}$$

In this case every measurement determines a semiaxis and of course T is evaluated as before via (29). Hence, as it is expected, if the orientation is known the number of measurements is reduced by three (the three Euler angles).

On the other hand, if the three semiaxes are known then m_0 is readily evaluated from (15) and (29). Also T is known from its expression (19), via (16). Hence, the eigenvalues of **M** are known, which in turn implies that the elements of the matrix **M** are connected through the known values of the three invariants of **M**, i.e., the trace $\lambda_1 + \lambda_2 + \lambda_3$, the determinant $\lambda_1\lambda_2\lambda_3$ and the second invariant $\lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_1$. Consequently, only three out of the six measurements m_k, $k = 1,2,...,6$, convey independent information about the orientation of the scatterer.

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Integrability of restricted multiple three-wave interactions

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Using a Hamiltonian framework with complex canonical variables allows for the determination of irreducible forms, which serve as building blocks for polynomial invariants. All the independent invariants in involution are thus obtained for the restricted multiple three-wave interactions, where all triads are coupled through a common pump (or daughter) wave, in the case of equal coupling strengths in all triads. The mixed, common pump/daughter wave case is not integrable.

I. INTRODUCTION

Nonlinear interactions between coherent waves or coupled oscillators can take place in many different physical systems, such as plasma physics, nonlinear optics, ocean wave dynamics, and many more. In the last decade, attention has been focused on the integrability or nonintegrability of the Hamiltonian equations describing the interactions between several wave triads, where each triad of coupled waves interacts with the other triads via one or possibly two common waves.[1–7]

As shown already elsewhere,[8] the sets of coupled-amplitude equations usually originate in complex notation and they can be studied with great advantage by using a Hamiltonian formalism, in which the complex conjugates of the wave amplitudes are also their canonically conjugated variables. The Hamiltonian remains a real quantity, in contrast to the recent study of integrable multiwave systems by Wojciechowski *et al.*,[7] who also use complex canonical variables.

Not only is the algebra greatly simplified, but one can use with great advantage the concept of irreducible forms to find in a rather systematic way the real invariants in involution needed to prove complete integrability, and this without having to resort to Lax operators, as was done by Menyuk *et al.*[5,6] or Wojciechowski *et al.*[7] These irreducible forms are the simplest combinations possible of wave quantities which remain constant on the fast oscillation time scale, and hence they can serve as building blocks in the construction of polynomial invariants on the slow modulation time scale.[9]

II. BASIC EQUATIONS FOR MANY COUPLED TRIADS WITH A COMMON PUMP WAVE

The nonlinear interaction between $2N+1$ waves is obtained by using a multiple time scale analysis[10] that separates the fast oscillations of each wave or oscillator from the slow modulation of its amplitude due to the nonlinear coupling between the different waves.

For simplicity, we will start from selection rules for the wave or oscillator frequencies, where the wave common to all triads is a so-called pump wave,

$$\omega_0 = \omega_m + \Omega_m + \delta_m \quad (m = 1,...,N), \tag{1}$$

with analogous relations for the wave vectors, if need be. Other cases of selection rules will be discussed further on.

In (1), δ_m is a small frequency mismatch or detuning. The complex amplitudes of the waves with frequencies ω_0, ω_m, and Ω_m $(m = 1,...N)$ are denoted by c, a_m, and b_m $(m = 1,...,N)$, and their slow-time variations are given by

$$\dot{a}_m = i\lambda_m c\bar{b}_m, \quad \dot{\bar{a}}_m = -i\lambda_m \bar{c} b_m,$$

$$\dot{b}_m = i\lambda_m c\bar{a}_m + i\delta_m b_m, \quad \dot{\bar{b}}_m = -i\lambda_m \bar{c} a_m - i\delta_m \bar{b}_m,$$

$$\dot{c} = i\sum_{m=1}^{N} \lambda_m a_m b_m, \quad \dot{\bar{c}} = -i\sum_{m=1}^{N} \lambda_m \bar{a}_m \bar{b}_m. \tag{2}$$

A different scaling on the wave amplitudes can put the frequency detuning into these equations in various ways, but (2) is about the simplest possible form. The dot refers to a derivative on the slow modulation time scale, and the bar to complex conjugation.

The set (2) is derivable from the Hamiltonian

$$H = \sum_{m=1}^{N} (\lambda_m (a_m b_m \bar{c} + \bar{a}_m \bar{b}_m c) + \delta_m b_m \bar{b}_m), \tag{3}$$

provided Hamilton's equations are written as[8]

$$\dot{a}_m = i\frac{\partial H}{\partial \bar{a}_m}, \quad \dot{b}_m = i\frac{\partial H}{\partial \bar{b}_m}, \quad \dot{c} = i\frac{\partial H}{\partial \bar{c}},$$
$$\dot{\bar{a}}_m = -i\frac{\partial H}{\partial a_m}, \quad \dot{\bar{b}}_m = -i\frac{\partial H}{\partial b_m}, \quad \dot{\bar{c}} = -i\frac{\partial H}{\partial c}. \tag{4}$$

The analysis of Menyuk *et al.*[5,6] showed that (2) is generically nonintegrable for arbitrary initial conditions and arbitrary frequency mismatches, except when all coupling constants λ_m are equal, in which case one can rescale all amplitudes so as to get $\lambda_m = 1$.

Menyuk *et al.*,[5] using the Painlevé criteria, also found a second case in which (2) would be integrable for arbitrary initial conditions, namely when

$$\lambda_1 = \cdots = \lambda_M = 2\lambda_{M+1} = \cdots = 2\lambda_N,$$
$$\delta_1 = \cdots = \delta_M = 2\delta_{M+1} = \cdots = 2\delta_N. \tag{5}$$

However, in this case the direct proof of integrability via a complete set of independent invariants in involution has so far eluded all efforts.

Finally, with perfect frequency tuning, one can select special initial conditions, making the value of H zero, and then the system described by (2) is integrable for arbitary λ_m (Ref. 3).

Here we will look at the restricted multiple three-wave interactions (2) with all $\lambda_m = 1$. The coupling is also restricted in the sense that the different triads share only a common wave, the same common wave in each triad.

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III. IRREDUCIBLE FORMS AND INDEPENDENT INVARIANTS IN INVOLUTION

In the Introduction, the irreducible forms have been described as the simplest real polynomial combinations of $a_m \exp i(\mathbf{k}_m \cdot \mathbf{x} - \omega_m t_{\text{fast}})$, $b_m \exp i(\mathbf{K}_m \cdot \mathbf{x} - \Omega_m t_{\text{fast}})$, $c \exp i(\mathbf{k}_0 \cdot \mathbf{x} - \omega_0 t_{\text{fast}})$, and their complex conjugates remaining invariant on the fast time scale. For a system such as (2), governed by selection rules (1), the irreducible forms are

$$a_m \bar{a}_m, \quad b_m \bar{b}_m, \quad c\bar{c}, \quad a_m b_m \bar{c} + \bar{a}_m \bar{b}_m c, \quad a_m b_m \bar{a}_p \bar{b}_p + \bar{a}_m \bar{b}_m a_p b_p. \tag{6}$$

All other real polynomial forms remaining constant with respect to the fast time scale (or the space scale, for that matter) are necessarily combinations of those mentioned in (6).

Irreducible forms as in (6) are usually not constant on the slow time scale, but suitable combinations can be invariant. Such invariants can be found by taking a closer look at the slow time derivatives of the irreducible forms and seeing how these can cancel.

The irreducible forms of the first line in (6) yield precisely $N+1$ independent Manley–Rowe relations or invariants, say one for each triad,

$$a_m \bar{a}_m = b_m \bar{b}_m + C_m, \tag{7}$$

besides a global one,

$$c\bar{c} + \sum_{m=1}^{N} b_m \bar{b}_m = E. \tag{8}$$

Through the correspondence between invariants or first integrals and symmetries of Hamiltonian systems,[11] these Manley–Rowe relations generate the following $(N+1)$-parameter group of transformations:

$$a_m = \hat{a}_m \exp i\epsilon_m, \quad b_m = \hat{b}_m \exp(i\epsilon - i\epsilon_m), \quad c = \hat{c} \exp i\epsilon, \tag{9}$$

which leave the set of equations (2) invariant. Since the $N+1$ Manley–Rowe relations are already in involution, one could attempt to extend them to a complete set of $2N+1$ first integrals in involution. If this can be done, the additional first integrals will automatically have to be invariant under the $(N+1)$-parameter transformation group (9). Real polynomials invariant under this group are precisely the irreducible forms given in (6) or combinations thereof. So it is entirely natural to look upon the irreducible forms as building blocks for additional polynomial invariants in involution.

Returning now to (6), one sees that the irreducible forms of the first line combine to the Hamiltonian (3).

Thus one starts for the other invariants from the irreducible forms $a_m b_m \bar{a}_p \bar{b}_p + \bar{a}_m \bar{b}_m a_p b_p$. To see how we proceed, let us call

$$H_m = a_m b_m \bar{c} + \bar{a}_m \bar{b}_m c + \delta_m b_m \bar{b}_m, \tag{10}$$

so that

$$H = \sum_{m=1}^{N} H_m, \tag{11}$$

with

$$\dot{H}_m = i \sum_{\substack{p=1 \\ p \neq m}}^{N} (a_p b_p \bar{a}_m \bar{b}_m - a_m b_m \bar{a}_p \bar{b}_p). \tag{12}$$

Similarly, setting

$$U_{mp} = \|a_m \bar{a}_p - \bar{b}_m b_p\|^2 = a_m \bar{a}_m a_p \bar{a}_p + b_m \bar{b}_m b_p \bar{b}_p - a_m b_m \bar{a}_p \bar{b}_p - a_p b_p \bar{a}_m \bar{b}_m, \tag{13}$$

which contain the last set of irreducible forms, one sees that

$$\dot{U}_{mp} = i(\delta_p - \delta_m)(a_m b_m \bar{a}_p \bar{b}_p - \bar{a}_m \bar{b}_m a_p b_p). \tag{14}$$

If all δ_m are different from each other, one gets immediately a set of N additional invariants.

$$I_m = H_m + \sum_{\substack{p=1 \\ p \neq m}}^{N} U_{mp} (\delta_p - \delta_m)^{-1}. \tag{15}$$

These correspond essentially to the invariants found earlier[6,7] by use of the Painlevé analysis and the Lax operator framework. However, as

$$H = \sum_{m=1}^{N} I_m = \sum_{m=1}^{N} H_m, \tag{16}$$

the Hamiltonian is functionally dependent upon the I_m. The system (2) is thus completely integrable, as we have $2N+1$ invariants (C_m, E, I_m) in involution, meaning that their Poisson brackets vanish. This last point can easily be checked.

If all δ_m are equal, it is clear from (14) that the U_{mp} themselves are $\frac{1}{2}N(N-1)$ additional independent invariants, besides the Manley–Rowe relations. Notice that

$$U_{mm} = C_m^2. \tag{17}$$

However, as the U_{mp} are not all in involution, it becomes necessary to group them in a proper way. This can be done in various equivalent ways, one of them being

$$K_m = \sum_{p=m+1}^{N} U_{mp}. \tag{18}$$

There are $N-1$ of these combinations, and now the $2N+1$ independent invariants in involution are (C_m, E, H, K_m).

For the intermediate cases, where some but not all frequency mismatches are equal, we proceed as follows.

Suppose first, to fix the ideas, that δ_1 and δ_2 are equal, but all the others mutually different. One cannot then use I_1 or I_2 as given in (15), but can take instead U_{12} and

$$I_{12} = H_1 + H_2 + \sum_{p=3}^{N} (U_{1p} + U_{2p})(\delta_p - \delta_1)^{-1} = \lim_{\delta_2 \to \delta_1} (I_1 + I_2), \tag{19}$$

and similarly for every pair of equal detunings.

Were three frequency mismatches to be equal, say $\delta_1 = \delta_2 = \delta_3$, then one replaces I_2, I_2, and I_3 by

$$I_{123} = H_1 + H_2 + H_3 + \sum_{p=4}^{N} (U_{1p} + U_{2p} + U_{3p})(\delta_p - \delta_1)^{-1}, \tag{20}$$

$$K_1' = U_{12} + U_{13}, \quad K_2' = U_{23}.$$

All possible choices of equal and unequal detunings can be dealt with in an analogous way. The new invariants in (19) or (20) are independent and in involution, with each other and with the others, with H as a dependent invariant.

IV. OTHER CASES AND FINAL REMARKS

In the above discussion we treated multiple three-wave couplings, where the one common wave was a pump wave in each triad.

The case of a common daughter wave in each triad is governed by the selection rules

$$\Omega_m = \omega_0 + \omega_m + \delta_m, \tag{21}$$

but runs entirely on analogous lines and will not be given here explicitly. Such systems have been proposed as models for internal ocean waves or plasma turbulence and are detailed elsewhere[1,6,7] via different methods.

Rather surprisingly, the mixed case where the common wave is a pump wave in some triads [with selection rules of type (1)] and a daughter wave in the others [with rules of type (21)] is qualitatively quite different, but seems to have been overlooked in previous studies.[6,7] For $N = 2$ it seems already nonintegrable, even when λ_1 and λ_2 are equal, and the addition of more triads will not improve matters.[9]

It is hoped that the above given treatment of restricted multiple three-wave couplings amply demonstrate the power of the combined method of a complex Hamiltonian formalism and irreducible forms. Although it was not detailed further for lack of space, the use of irreducible forms also directly points out that all λ_m have to be equal if integrability is to exist.

The fact that the other case, where the couplings and the detunings obey (5) and which was also surmised by Menyuk *et al.*[5] to be integrable, so far seems intractable could perhaps be an indication that its missing invariant (or invariants) cannot be a simple polynomial.

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Quantum observables: Compatibility versus commutativity and maximal information

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Two different approaches to a characterization of the degree of (in)compatibility of quantum observables are investigated. First, recent examples of the (partial) commutativity of spectral measures of incompatible observables are proved to be generic. The analysis is extended to the case of compatible or incompatible unsharp, or stochastic observables, leading to a general criterion for commutativity of position and momentum effects. Further, a recently proposed information theoretic quantification of the (in)compatibility of noncommuting observables is generalized, and the relation between "maximal information," "minimal uncertainty," partial commutativity, and strict correlation is further clarified. Both approaches are illustrated in a number of examples.

I. INTRODUCTION

This work contributes to a more refined understanding of the operational content of noncommutativity of quantum observables. It is well known that noncommutativity is equivalent to incompatibility in the case of *sharp* observables represented by projection-valued (PV) measures.[1] On the other hand, the so-called *unsharp*, or *stochastic* observables [represented by effect-valued, also called positive-operator-valued (POV) measures] may be compatible, or coexistent (that is, admit joint observables) without being commutative.[2] Recent investigations have shown that the degree of noncommutativity can be quantified; for example, the incompatible sharp position and momentum observables possess pairs of spectral projections which are either totally noncommutative, or partially commutative, or even commutative.[3] The underlying characterization of the degree of (non)commutativity can be extended to the case of stochastic observables. This is the subject of Sec. II where the most general criterion for the commutativity of position and momentum effects is given. We show that the introduction of unsharpness does not necessarily change the degree of noncommutativity. Thus all POV measures representing (unsharp) position and momentum have different choices of arguments (Borel sets) for which they partially or totally commute, for other choices do not commute, and still are coexistent in the sense of having joint observables. We conclude that commutativity is not an ideal characterization of compatibility (simultaneous observability) of observables. We turn to an alternative quantitative measure concerning simultaneous measurability, namely a quantification of the indeterminacy of the simultaneous measurement of any observables.

Noncommuting observables cannot be simultaneously determined with arbitrary accuracy; there must in general be a certain amount of indeterminacy, no matter what measure of the spread is used. This fact raises the question as to how much *information* can simultaneously be available about those observables. In Ref. 4 several functionals $\mathcal{F}[\phi] = f(\langle E\rangle_\phi, \langle F\rangle_\phi)$ expressible as functions of the expectation values of effects E, F in state ϕ were studied as potential measures of (maximal) information. Here (Sec. III) the maximization of a general class of functionals will be investigated in some detail, leading to a clarification of the relation between "maximal information" and "minimal uncertainty." In particular, maximal information in whatever sense requires the vanishing of the expectation of the commutator and equality in the uncertainty relation, that is, strict correlation for that maximal information state. Thus commutativity in the expectation value arises as a consequence of a general information analysis.

In Sec. IV the main conclusions will be summarized.

II. DEGREE OF NONCOMMUTATIVITY

For pairs of Hilbert space projections P, Q the degree of noncommutativity can be described in terms of the "commutativity projection"

$$\mathrm{com}(P,Q) = (P\wedge Q)\vee(P\wedge Q^\perp) \vee(P^\perp\wedge Q)\vee(P^\perp\wedge Q^\perp) \tag{1}$$

($P\wedge Q$, $P\vee Q$ denoting the projectors onto the intersection, union of the ranges of P and Q, respectively, $P^\perp = \mathbf{1} - P$, etc.). The operator $\mathrm{com}(P, Q)$ is the projector onto the subspace of vectors on which P and Q do commute. This formulation can immediately be extended to the class of effects E, F ($0\leqslant E, F\leqslant \mathbf{1}$, that is, E and F have spectra within the interval $[0, 1]$): $\mathrm{com}(E, F)$ projects onto the subspace of states on which E and F are commutative, that is,

$$\mathrm{com}(E,F)H = \{\phi\in H \mid (EF - FE)\phi = [E,F]\phi = 0\}. \tag{1'}$$

Then one may call E, F *commutative* if $\mathrm{com}(E,F) = \mathbf{1}$, *partially* (non)*commutative* if $0\neq\mathrm{com}(E,F)\neq\mathbf{1}$, and (*totally*) *noncommutative* if $\mathrm{com}(E,F) = 0$. In Ref. 3 examples of pairs of position and momentum spectral projections $E^Q(X)$, $E^P(Y)$ were given for each category. Here Q and P

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may be introduced as any (irreducible) representation of the Weyl commutation relation; that is, Q, P may be any Fourier couple. For technical reasons, such as the use of Fourier transformations, one employs the Schrödinger representation. Then the results of Ref. 3 can be extended to unsharp position and momentum observables, defined as POV measures through the following:

$$\begin{aligned} a_\nu^Q(X) &= \int_{\mathbf{R}} d\nu(q) E^Q(X+q) \\ &= \int_{\mathbf{R}} dE^Q(q)(\nu * \chi_X)(q) = (\nu * \chi_X)(Q), \\ a_{\nu'}^P(Y) &= \int_{\mathbf{R}} d\nu'(p) E^P(Y+p) \\ &= \int_{\mathbf{R}} dE^P(p)(\nu' * \chi_Y)(p) = (\nu' * \chi_Y)(P), \end{aligned} \tag{2}$$

where ν, ν' are normalized, positive *confidence* (Borel) measures, $X, Y \in B(\mathbf{R})$. Thus

$$\begin{aligned} C(X,Y) \equiv [a_\nu^Q(X), a_{\nu'}^P(Y)] &= \iint_{\mathbf{R}^2} d\nu(q) d\nu'(p) \\ &\times [E^Q(X+q), E^P(Y+p)]. \end{aligned} \tag{3}$$

Now one may readily translate some of the results obtained in Ref. 3 for the spectral projections.

It has been shown in Ref. 3 that $E^Q(X), E^P(Y)$ may be (i) totally noncommutative, e.g., for X, Y being half-lines; (ii) partially commutative, e.g., for X, Y being bounded Borel sets; (iii) commutative for (X,Y) being α-periodic, that is, $(X,Y) = (X+\alpha, Y+2\pi/\alpha)$ for some positive constant α.

From the above expression for $C(X,Y)$ it is seen that commutativity holds for arbitrary measures ν, ν' if (X,Y) is α-periodic: in that case also $(X+q, Y+p)$ is α-periodic for arbitrary q, p. Now let us assume ν, ν' to have bounded supports $[-a,a]$ and $[-b,b]$, respectively. Let $X = [-x_0, x_0]$, $Y = [-y_0, y_0]$ and define $X^a = [-x_0 - a, x_0 + a]$, $Y^b = [-y_0 - b, y_0 + b]$. Then $X + q \subseteq X^a$, $Y + p \subseteq Y^b$ for $q \in \operatorname{supp} \nu$, $p \in \operatorname{supp} \nu'$, so

$$\begin{aligned} E &= E^Q(\mathbf{R} \setminus X^a) \wedge E^P(\mathbf{R} \setminus Y^b) \\ &\leqslant E^Q(\mathbf{R} \setminus X + q) \wedge E^P(\mathbf{R} \setminus Y + p), \end{aligned}$$

for all $q \in \operatorname{supp} \nu$, $p \in \operatorname{supp} \nu'$; and all eigenvectors of E will be eigenvectors of all $E^Q(X+q)$, $E^P(Y+p)$. Thus $C(X,Y)\phi = 0$ on the subspace $E\mathcal{H}$, that is, $a_\nu^Q(X)$ and $a_{\nu'}^P(Y)$ are partially commutative. (We will argue below that these effects are not commutative.) Next, if X, Y are half-lines, supp ν and supp ν' bounded, then $a_\nu^Q(X)$, $a_{\nu'}^P(Y)$ are totally noncommutative because $E^Q(X)$ and $E^P(Y)$ are: the supports of $a_\nu^Q(X)$ and $a_{\nu'}^P(Y)$ are half-lines again so that the intersection of their ranges is $\{0\}$; this holds for all pairs $(a_\nu^Q(X^i), a_{\nu'}^P(Y^j))$ with $X^i \in \{X, \mathbf{R} \setminus X\}$, $Y^j \in \{Y, \mathbf{R} \setminus Y\}$ so that there is no common range at all.

The last two examples rest on the assumption of compact supports for ν, ν'; the introduction of more general kinds of unsharpness (confidence measures) seems to decrease the extent of partial commutativity. On the other hand, it is the introduction of unsharpness that opens the possibility of compatible position and momentum observables,[2,5] and it is necessary to avoid compact support of at least one of the measures ν, ν' for achieving compatibility. Take absolutely continuous measures $d\nu(q) = f(q)dq$, $d\nu'(p) = g(p)dp$, where $f(q) = |\psi_0(q)|^2$, $g(p) = |\hat{\psi}_0(p)|^2$, for $\psi_0 \in L^2(\mathbf{R})$. Then a_ν^Q, $a_{\nu'}^P$ are marginals of the phase space observable

$$\begin{aligned} Z \mapsto A(Z) &= \iint_Z dq\, dp |\psi_{qp}\rangle\langle\psi_{qp}|, \quad Z \in B(\mathbf{R}^2), \\ \psi_{qp} &= \exp[i(-qP + pQ)]\psi_0, \end{aligned} \tag{4}$$

and therefore are coexistent although they do not commute in general. The opposite will also occur: for compactly supported measures and bounded sets X, Y the effects $a_\nu^Q(X)$, $a_{\nu'}^P(Y)$ possess no joint observable, but these effects do partially commute as was shown above. This confirms the conclusion of Ref. 2 that commutativity is not essential to coexistence (compatibility) in case of stochastic observables.

We now generalize the α-periodicity condition slightly to get a necessary and sufficient condition for commutativity. For this we consider the following.

Let ν, ν' be positive normalized Borel measures and define

$$\nu_X = \nu * \chi_X, \quad \nu'_Y = \nu' * \chi_Y, \quad \text{for } X, Y \in B(\mathbf{R});$$

that is,

$$\nu_X(q) = \int d\nu(y) \chi_X(q-y) \text{ a.e., etc.}$$

Then $\nu_X, \nu_Y \in L^\infty(\mathbf{R}, dq)$. If we also let $\mathcal{F}$ ($\mathcal{F}^{-1}$) denote (inverse) Fourier transform in $L^2(\mathbf{R}, dq)$ and working in the Schrödinger representation for Q, P, we then have, for unsharp observables,

$$\begin{aligned} C(X,Y)\phi &\equiv [a_\nu^Q(X), a_{\nu'}^P(Y)]\phi \\ &= \nu_X \mathcal{F}^{-1}[\nu'_Y \mathcal{F}(\phi)] \\ &\quad - \mathcal{F}^{-1}[\nu'_Y \mathcal{F}(\nu_X \phi)], \end{aligned} \tag{5}$$

for all $\phi \in L^2(\mathbf{R}, dq)$. Since $f \in L^\infty$, $g \in L^2$ implies $fg \in L^2$, this defines $C(X,Y)$ as a mapping on L^2. A complete characterization of $C(X,Y) = 0$ is given by the following theorem the proof of which can be found in the Appendix.

Theorem 1: Let $f, g \in L^\infty(\mathbf{R}, dq)$. Then

$$f\mathcal{F}^{-1}[g\mathcal{F}(\phi)] = \mathcal{F}^{-1}[g\mathcal{F}(f\phi)] \tag{6}$$

holds for all $\phi \in L^2(\mathbf{R}, dq)$ if and only if f and g satisfy one of the following: (a) at least one of f or g is constant a.e.; or (b) f and g are both periodic with minimal periods β, α satisfying $2\pi/\alpha\beta \in \mathbf{Z} \setminus \{0\}$ ("generalized α-periodicity").

We remark that case (a) is of little interest here since we identify $f = \nu_X$, $g = \nu'_Y$. If we have either constant, this leads to one of $a_\nu^Q(X)$, $a_{\nu'}^P(Y)$ being a multiple of the identity. The case (b) with ν, ν' taken as point measures (delta measures) generalizes the known results for sharp observables.[3] For the general case, consider

$$\nu_X(q) = \nu_X(q+\beta) \text{ a.e. } q$$

iff

$$\int d\nu(y)\chi_X(q-y) = \int d\nu(y)\chi_X(q+\beta-y) \text{ a.e. } q$$

iff

$$\nu(-X+q) = \nu(-X+q+\beta) \text{ a.e. } q$$

iff

$$\nu((-X/(-X+\beta))+q) = \nu((-X+\beta)/X+q) \text{ a.e. } q,$$

from which we see that periodicity of X leads to periodicity of ν_X. We therefore obtain a second derivation of commutativity of the *unsharp* observables from the (generalized) α-periodicity of (X,Y). We also note that there are no solutions $\nu_X \neq 0$ for X essentially bounded or essentially semi-infinite since this leads to a contradiction to ν being a normalized positive measure.

In view of the one-to-one correspondence between L^∞ functions f,g and bounded operator functions of position and momentum,

$$f(Q) = \int_{\mathbf{R}} f(q)dE^Q(q), \quad g(P) = \int_{\mathbf{R}} g(p)dE^P(p), \quad (7)$$

Eq. (6) can be rewritten as

$$[f(Q),g(P)] = 0 \quad (8)$$

which holds in any Hilbert space representation of the canonical commutation relations if and only if one of the following is satisfied: (a) at least one of $f(Q), g(P)$ is a multiple of the identity operator, and (b) f and g are both periodic with minimal periods β,α satisfying $2\pi/\alpha\beta \in \mathbf{Z}\setminus\{0\}$.

III. INFORMATION MAXIMIZATION

In Ref. 4 various measures of "joint information" for (expected values of) pairs of effects E,F have been studied with regard to their maximization. The first variation (in the sense of the Fréchet differential[6]) of the functional $\mathcal{F}[\phi] = f(\langle E\rangle_\phi, \langle F\rangle_\phi)$ with respect to $\phi \in \mathcal{H}$ is given by

$$\mathcal{F}[\phi+\delta\phi] - \mathcal{F}[\phi] = \delta\mathcal{F}[\delta\phi;\phi] + \epsilon[\delta\phi],$$

where $\delta\mathcal{F}$ must be a continuous linear functional in $\delta\phi$ and $\lim_{||\delta\phi||\to 0}(\epsilon[\delta\phi]/||\delta\phi||) = 0$. Here $\mathcal{F}$ will be locally extremal on a vector ϕ with $||\phi|| = 1$ only if

$$\delta(\mathcal{F} + \lambda\langle\phi|\phi\rangle) = 0,$$

which implies

$$0 = (f_1E + f_2F + \lambda\mathbf{1})\phi, \quad (9)$$

where $f_i = (\partial f/\partial x_i)(\langle E\rangle_\phi, \langle F\rangle_\phi)$ $(i = 1,2)$. The Lagrange parameter is found by taking the expectation

$$\lambda = -f_1\langle E\rangle_\phi - f_2\langle F\rangle_\phi;$$

therefore Eq. (1) can be written as

$$\begin{aligned} 0 &= (f_1E' + f_2F')\phi, \\ E' &= E - \langle E\rangle_\phi\mathbf{1}, \quad F' = F - \langle F\rangle_\phi\mathbf{1}. \end{aligned} \quad (10)$$

Multiplying this equation either with E' or with F' and taking the expectation yields the system

$$\begin{aligned} 0 &= f_1\langle E'^2\rangle_\phi + f_2\langle E'F'\rangle_\phi, \\ 0 &= f_1\langle F'E'\rangle_\phi + f_2\langle F'^2\rangle_\phi. \end{aligned} \quad (11)$$

Here f_1 and f_2 are fixed as partial derivatives of f; so in order to have local extrema for $\mathcal{F}$ one must have either $f_1 = f_2 = 0$ or have the vanishing of the determinant,

$$\mathrm{Var}_\phi(E)\cdot\mathrm{Var}_\phi(F) - |\langle E'F'\rangle_\phi|^2 = 0. \quad (12)$$

In that latter case one solves (assuming $f_2 \neq 0$)

$$\frac{f_1}{f_2} = -\frac{\langle E'F'\rangle_\phi}{\mathrm{Var}_\phi(E)} = -\frac{\mathrm{Var}_\phi(F)}{\langle F'E'\rangle_\phi} = \pm\left[\frac{\mathrm{Var}_\phi(F)}{\mathrm{Var}_\phi(E)}\right]^{1/2}. \quad (13)$$

Here we have assumed f to be real. If $f_2 = 0$ then either $f_1 = 0$ or $\mathrm{Var}_\phi(E) = 0$, i.e., $E'\phi = 0$. Therefore we may separate the "trivial" solutions corresponding to $f_1 = f_2 = 0$ (local extremum of f), or $f_1 = 0$, $F'\phi = 0$, or $f_2 = 0$, $E'\phi = 0$, or $F'\phi = E'\phi = 0$, and the remaining solutions of (10) have to satisfy (12) and (13).

These connections can be generalized in several respects, as we shall see in the following theorems. In particular, we shall consider functionals not only on the Hilbert space of pure states but also try to include mixed states. The most natural way of extending the above derivations to this general class of states turns out to be in terms of the Hilbert Schmidt class $B_2(H)$; the choice of the trace class $B_1(H)$ leads to trivial results only.

We shall first prove the following.

Theorem 2: Let $\mathcal{F}$ be a real-valued functional on $B_2(H)$ such that $\mathcal{F}[r] = f(\langle A_1\rangle_\rho, ..., \langle A_n\rangle_\rho)$, A_i bounded self-adjoint operators, $\rho = rr^*$, $r \in B_2(H)$ [so ρ is a positive element in $B_1(H)$], $\langle A_i\rangle_\rho = \mathrm{Tr}[\rho A_i] = (r, A_i r)$, f differentiable. Then $\mathcal{F}$ is Fréchet differentiable. In particular, if $\mathcal{F}$ has a local extremum on $r = \rho^{1/2}$ under the constraint $\mathrm{Tr}|\rho| = (r,r) = 1$, then the first Fréchet variation vanishes, $0 = \delta(\mathcal{F} + \lambda\,\mathrm{Tr}[\rho])$, which implies

$$0 = \sum_i f_i(A_i - \langle A_i\rangle_\rho\mathbf{1})\cdot\rho^{1/2}, \quad (14)$$

where

$$f_i = \frac{\partial f}{\partial x_i}(\langle A_1\rangle_\rho, ..., \langle A_n\rangle_\rho),$$

or, equivalently,

$$0 = \sum_i f_i(A_i - \langle A_i\rangle_\rho\mathbf{1})\phi, \quad \text{for all } \phi \text{ in the range of } \rho. \quad (15)$$

Proof: The Fréchet differentiability of $\mathcal{F}$ is shown by a straightforward but gory computation. The Fréchet differential of $\mathcal{F}$ is

$$\delta\mathcal{F}[\delta r;r] = \sum_i f_i[(r,A_i\delta r) + (\delta r, A_i r)].$$

It is linear, i.e., $\delta\mathcal{F}[h+k;r] = \delta\mathcal{F}[h;r] + \delta\mathcal{F}[k;r]$, and bounded with respect to the $B_2(H)$ norm ($||r||_2 = (r,r)^{1/2} = \{\mathrm{Tr}[r^*r]\}^{1/2}$):

$$|\delta\mathcal{F}[\delta r;r]| \leq \left\{2\sum_i |f_i|\,||A_i||\right\}||\delta r||_2.$$

Then for a local extremum of $\mathcal{F}$ one has

$$0=\delta(\mathcal{F}+\lambda\,\mathrm{Tr}[\rho])=\left(\delta r,\left\{\sum_i f_iA_i+\lambda\mathbb{1}\right\}r\right)+\text{c.c.},$$

which yields, due to the arbitrariness of $r\in B_2(H)$,

$$0=\left\{\sum_i f_iA_i+\lambda\mathbb{1}\right\}\cdot\rho^{1/2}.$$

The Lagrange parameter λ is found by evaluation of the condition $1=\mathrm{Tr}[\rho]=(r,r)$:

$$\lambda=-\sum_i f_i\langle A_i\rangle_\rho.$$

The remaining step is straightforward since for bounded A, $A\rho^{1/2}=0$ is equivalent to $A\rho=0$ and also to $A\phi=0$ for all ϕ in the range of ρ. This completes the proof.

At first sight it appears surprising that all vectors in the range of the maximizing ρ satisfy the same equation (15). However, this simply means that the pure states maximizing the functional $\mathcal{F}$ span a closed subspace which is an eigenspace of the bounded linear operator $\Sigma_{i=1}^n f_iA_i$.

Theorem 3: The coefficients α_i in the (linear in ϕ) equation $0=(\Sigma_i\alpha_iA_i+\lambda\mathbb{1})\phi$, or equivalently (in the nonlinear equation) $\Sigma_i\alpha_iA_i'\phi=0$ $(A_i'=A_i-\langle A_i\rangle_\phi)$, are determined as functions $\alpha_i=g_i(\langle A_k'A_l'\rangle_\phi;\gamma_j)$ of the (complex) covariances $\langle A_k'A_l'\rangle_\phi$ and r parameters γ_j where $n-r$ is the rank of the matrix $(\langle A_k'A_l'\rangle_\phi)$. A nontrivial set $(\alpha_1,\ldots,\alpha_n)\neq(0,\ldots,0)$ requires $\det(\langle A_k'A_l'\rangle_\phi)=0$.

Proof: Multiplying the equation with A_k', $k=1,\ldots,n$, and taking the expectation yields the system

$$\sum_{l=1}^n\alpha_l\langle A_k'A_l'\rangle_\phi=0,\quad k=1,\ldots,n.$$

The remainder is a simple application of linear algebra.

The case $n=1$ has a nontrivial solution iff $\mathrm{Var}_\phi(A_1)=0$; that is, ϕ is an eigenvector of A_1. The case $n=2$ has been solved completely in Ref. 7 with the following result.

Theorem 4: In the uncertainty relation (Cauchy–Schwarz inequality) for self-adjoint A, B,

$$\begin{aligned}&\mathrm{Var}_\rho(A)\cdot\mathrm{Var}_\rho(B)\\&\quad\equiv\langle A'^2\rangle_\rho\langle B'^2\rangle_\rho\geqslant|\langle A'B'\rangle_\rho|^2\\&\quad=|\tfrac{1}{2}\langle[A,B]\rangle_\rho|^2+(\tfrac{1}{2}\langle\{A',B'\}_+\rangle_\rho)^2\end{aligned}\tag{16}$$

equality is obtained if and only if $\mathrm{Var}_\rho(B)=0$ or $\mathrm{Var}_\rho(B)\neq0$ and $[A'-(\langle B'A'\rangle_\rho/\mathrm{Var}_\rho(B))B']\rho^{1/2}=0$. This latter condition is equivalent to

$$0=[A'-(\langle B'A'\rangle_\rho/\mathrm{Var}_\rho(B))B']\rho,\tag{17}$$

or

$$0=[A'-(\langle B'A'\rangle_\rho/\mathrm{Var}_\rho(B))B']\phi,\quad\text{for all }\phi\text{ in the range of }\rho.\tag{18}$$

So we arrive at just the "linear" equation obtained earlier from the maximization of $f(\langle E\rangle_\phi,\langle F\rangle_\phi)$ [cf. Eq. (10)].

We summarize and combine the above statements.

Theorem 5: A real functional $\mathcal{F}[r]=f(\langle A_1\rangle_\rho,\ldots,\langle A_n\rangle_\rho)$, $\rho=rr^*$, $r\in B_2(H)$, with f and self-adjoint bounded A_i such that $\mathcal{F}$ is Fréchet differentiable will be locally extremal only on states ρ satisfying

$$\sum_{i=1}^n f_i(A_i-\langle A_i\rangle_\rho\mathbb{1})\rho=0\tag{19}$$

and for $(f_1,\ldots,f_n)$ obeying

$$\sum_{i=1}^n f_i\langle A_k'A_i'\rangle_\rho=0,\tag{20}$$

where either $f_1=\cdots=f_n=0$ or $\det(\langle A_k'A_i'\rangle_\rho)=0$.

The solutions of these equations yield extrema of $\mathcal{F}$ iff at $(x_1,\ldots,x_n)=(\langle A_1\rangle_\rho,\ldots,\langle A_n\rangle_\rho)$ the function f is extremal on the numerical range of $A_1,\ldots,A_n$,

$$\begin{aligned}&\text{num ran}(A_1,\ldots,A_n)\\&\quad=\{(x_1,\ldots,x_n)\,|\,x_i=\langle A_i\rangle_\rho,\\&\qquad\rho\text{ any positive trace 1 operator}\}.\end{aligned}$$

Consequences: (i) For $n=1$ the only possible solutions are $(\partial f/\partial x)(\langle A\rangle_\rho)=0$ or $\mathrm{Var}_\rho(A)=0$, that is, ρ is an "eigenstate" of A.

(ii) For $n=2$, either ρ is a common eigenstate of A, B, or $f_1=f_2=0$ on ρ, or $\mathrm{Var}_\rho(A)=0$ and $f_2=0$, or $\mathrm{Var}_\rho(B)=0$ and $f_1=0$, or $\mathrm{Var}_\rho(a)\neq0\neq\mathrm{Var}_\rho(B)$ and

$$\frac{f_1}{f_2}=-\frac{\langle A'B'\rangle_\rho}{\mathrm{Var}_\rho(A)}=-\frac{\mathrm{Var}_\rho(B)}{\langle B'A'\rangle_\rho}=\pm\left[\frac{\mathrm{Var}_\rho(B)}{\mathrm{Var}_\rho(A)}\right]^{1/2}\tag{21}$$

and

$$\mathrm{Var}_\rho(A)\mathrm{Var}_\rho(B)=\tfrac{1}{4}(\langle\{A',B'\}_+\rangle_\rho)^2=[\mathrm{cov}_\rho(A,B)]^2.\tag{22}$$

In particular, the reality of f_1,f_2 forces $\langle A'B'\rangle_\rho$ to be real so that only the covariance term appears in (22), and

$$\langle[A,B]_-\rangle_\rho=0\quad\text{on any extremalizing state }\rho.\tag{23}$$

Equation (22) tells that in such states ρ the observables A, B are strictly (anti-)correlated, $\mathrm{corr}_\rho(A,B)=\pm1$.

With these results we arrive at a generalization and a complete clarification of the relationships (9)–(13) reviewed in the beginning of this section which had been found earlier[4] in some examples. Furthermore, we obtain a means for comparing the various possible measures of information insofar as different functions $f(x,y)$ admit different solutions for possible extrema. This will be illustrated in a number of examples. First we consider pairs of projections P, Q, so that num ran$(P,Q)\subseteq[0,1]\times[0,1]$, and the unit square will be the natural domain of our functions $f(x,y)$.

Example 1:

$$\begin{aligned}f(x,y)=&\,x\ln x+(1-x)\ln(1-x)+y\ln y\\&+(1-y)\ln(1-y).\end{aligned}$$

Here

$$I_\phi(Q)=\langle Q\rangle_\phi\ln\langle Q\rangle_\phi+\langle\mathbb{1}-Q\rangle_\phi\ln\langle\mathbb{1}-Q\rangle_\phi$$

represents the (missing) information about Q in state ϕ in the sense of negative entropy, and

$$I_\phi(Q,P)=I_\phi(Q)+I_\phi(P)=f(\langle Q\rangle_\phi,\langle P\rangle_\phi)$$

is a measure of the information simultaneously available on

Q and P. Now $f_1 = \ln[x/(1-x)], f_2 = \ln[y/(1-y)]$, and $f_1 = f_2 = 0$ if and only if $x = y = \frac{1}{2}$ which is known to yield the absolute minimum $-2\ln 2$ of f and thus of $\mathscr{F}[\phi] = I_\phi(Q,P)$. The absolute maximum 0 of f is assumed on $(x,y) \in \{(0,0), (0,1), (1,0), (1,1)\}$, which can be realized by $(\langle P\rangle_\phi, \langle Q\rangle_\phi)$ if and only if there exist joint eigenstates. Thus it depends on the degree of commutativity whether or not the information can be absolutely maximal or not.

The variance of a projection is $\mathrm{Var}_\phi(P) = \langle P\rangle_\phi - \langle P\rangle_\phi^2$ so that condition (21) on f_1/f_2 reads

$$[x(1-x)]^{1/2}\ln[x/(1-x)] = \pm [y(1-y)]^{1/2}\ln[y/(1-y)]$$

or

$$\Psi(x) = \Psi(y)^{\pm 1}, \quad \Psi(x) = (x/(1-x))^{[x(1-x)]^{1/2}},$$

where by continuity $\Psi(0) = \Psi(1) = 1$. Noting $\Psi(0) = \Psi(\frac{1}{2}) = \Psi(1) = 1$ and that Ψ has a minimum on $x_0 \in (0,\frac{1}{2})$ and a maximum on $x_1 \in (\frac{1}{2},1)$ and satisfies $\Psi(1-x) = \Psi(x)^{-1}$, one obtains exactly four solutions $y = x$, $y = 1-x$, $y = x^*$, and $y = 1-x^*$, where x and x^* are the solutions of $\Psi(x) = u$ for u in the range of Ψ (for $x = x_0$ or $x = x_1$ it follows that $x = x^*$, so in that case there are only two solutions).

Example 2: $f(x,y) = x + y$. Here $\mathscr{F}[\phi] = \langle P\rangle_\phi + \langle Q\rangle_\phi$ is the sum of probabilities. Then $f_1 = f_2 = 1$, so Eq. (21) yields

$$1 = f_1/f_2 = [y(1-y)/x(1-x)]^{1/2},$$

which has $y = x$ and $y = 1-x$ as the only solutions.

Example 3: $f(x,y) = x\cdot y$ corresponds to the product of probabilities. Here $f_1 = y, f_2 = x$. The absolute minimum occurs on $x = 0$ or $y = 0$. Otherwise [Eq. (21)]

$$f_1/f_2 = y/x = [y(1-y)/x(1-x)]^{1/2}$$

or

$$[(1-x)/x]^{1/2} = [(1-y)/y]^{1/2}$$

with $y = x$ as the only solution.

Example 4: $f(x,y) = x(1-x)\cdot y(1-y)$ corresponds to $\mathscr{F}[\phi] = \mathrm{Var}_\phi(P)\cdot\mathrm{Var}_\phi(Q)$. Here $f_1 = (1-2x)\times y(1-y), f_2 = x(1-x)(1-2y)$, and $f_1 = 0$ iff $x = \frac{1}{2}$ or $y \in \{0,1\}$. Thus the absolute minimum 0 of f occurs on the eigenstates of P,Q, the absolute maximum on $x = y = \frac{1}{2}$. If neither is the case, (21) yields

$$\Psi(x) \equiv [x(1-x)]^{1/2}/(1-2x) = \pm\Psi(y)$$

with $\Psi(1-y) = -\Psi(y)$, $\Psi'(x) > 0$. So the only solutions are $y = x$ and $y = 1-x$.

In all of these examples the solutions $y = x$ (and $y = 1-x$) lead to (local) extrema if the boundary points (x,y) of num ran(P,Q), satisfying $y = x$ (or $y = 1-x$) belong to the set num ran(P,Q). We see that the number of possible extrema depends essentially on the degree of symmetry of the functions f ($f(x,y) = f(y,x)$; $f(1-x,y) = f(x,y)$, etc.) as well as on the shape of the (convex) numerical range of P,Q. We remark that Lenard[8] gives an exhaustive description of num ran(P,Q) so that in principle all extrema of functionals $\mathscr{F}[\phi] = f(\langle P\rangle_\phi, \langle Q\rangle_\phi)$ can actually be determined.

Example 5: The final example deals with a more complicated functional,

$$\begin{aligned}\mathscr{F}[\phi] &= \mathrm{Var}_\phi(A)\cdot\mathrm{Var}_\phi(B)\\ &= (\langle A^2\rangle_\phi - \langle A\rangle_\phi^2)(\langle B^2\rangle_\phi - \langle B\rangle_\phi^2)\\ &= f(\langle A\rangle_\phi, \langle B\rangle_\phi, \langle A^2\rangle_\phi, \langle B^2\rangle_\phi).\end{aligned}$$

Application of Theorem 2 yields for the extremal states,

$$0 = [\mathrm{Var}_\phi(B)(A^2 - 2\langle A\rangle_\phi A) + \mathrm{Var}_\phi(A)(B^2 - 2\langle B\rangle_\phi B) + \lambda\mathbb{1}]\phi;$$

since $A'^2 - \langle A\rangle_\phi^2\mathbb{1} = A^2 - 2\langle A\rangle_\phi A$, etc., this equation can be brought into the form

$$0 = [\mathrm{Var}_\phi(B)A'^2 + \mathrm{Var}_\phi(A)B'^2 - 2\,\mathrm{Var}_\phi(A)\cdot\mathrm{Var}_\phi(B)\mathbb{1}]\phi.$$

Possible solutions are eigenstates of A or B; further solutions will be found by observing that this equation is precisely an instance of the case $n = 2$ in Theorems 4 and 5, leading to Eqs. (21)–(23). In particular, Eq. (23) reads

$$\langle [A'^2, B'^2]_-\rangle_\phi = 0.$$

If we insert for A,B the position Q and momentum P operators (although they are not bounded), then

$$[Q'^2, P'^2]_- = 2i\hbar\{Q', P'\}_+$$

so $\langle [Q'^2, P'^2]_-\rangle_\phi = 0$ if and only if $\langle \{Q', P'\}_+\rangle_\phi = 0$ which singles out the coherent (Gaussian) states of minimal uncertainty.

IV. CONCLUDING REMARKS

In Sec. II we constructed examples of generalized, unsharp position and momentum observables whose effects $a_\nu^Q(X), a_\nu^P(Y)$ may be either totally noncommutative, or partially commutative, or commutative. We established a characterization of the commutative case: $[a_\nu^Q(X), a_\nu^P(Y)] = 0$ whenever (X,Y) is α-periodic, $(X,Y) = (X+\alpha, Y+2\pi/n\alpha)$ for some fixed $\alpha > 0$. For the investigation of partial commutativity the question of positive lower bounds[9] $a \leqslant a_\nu^Q(X), a_\nu^P(Y)$ may be of relevance, as it is in the case of projections.

One possibility of introducing approximate measurements of noncommuting observables A, B within conventional quantum mechanics is in terms of joint measurements of commuting functions $f(A), g(B)$ of A,B. Then Theorem 1 tells that the only approximate joint measurements of Q,P in this sense are those by means of (generalized) α-periodic functions f,g (as long as only bounded functions are considered). In contrast, after introducing POV observables commutativity is no longer necessary (though still sufficient) for coexistence so that much more flexiblity is gained.

These results show that "commutativity" and "compatibility" are quite unrelated in general from the mathematical standpoint. This is also true from the viewpoint of measurement theory.[2] There are compatible observables that do not commute; the "price" to be paid for obtaining coexistence "in spite" of noncommutativity is unsharpness, that is, lack of certainty inherent in the results of joint measurements.

This lack of certainty can be estimated in the way indicated in Sec. III, by searching for maxima of "information" functionals $\mathscr{F}[\phi] = f(\langle A_1\rangle_\phi,\ldots,\langle A_n\rangle_\phi)$. It turns out that optimal upper and lower bounds for the information are determined by the extrema of f on the numerical range of $(A_1,\ldots,A_n)$. In particular, for $n=2$ extrema occur only on strictly correlated states with vanishing expectation of the commutator. This means that on any state of maximal information, in the sense defined here, the variances have to be finite. Thus at least in this respect the usefulness of the variances as uncertainty measures is supported.[10]

According to Theorem 2, the information maximizing states ϕ satisfy an equation of the form [Eq. (15)] $\Sigma_i f_i A_i \phi = \lambda 1\phi$. In the context of $U(n)$ representations with A_i being self-adjoint generators of infinitesimal unitary transformations, this equation generalizes the statement that ϕ is a highest weight state.[7]

For pairs of projections P, Q we found the locations of the solutions of the variational equations in the case of several functions f. The examples show that functions of the form $f(x,y) = g(x) + g(y)$ (examples 1 and 2) are more suitable for the description of uncertainty than $f(x,y) = h(x)\cdot h(y) > 0$ (examples 3 and 4): in the latter type minimal uncertainty in the case of small h remains quite undetermined since the minimum 0 occurs if only one factor is zero. The symmetry $f(x,y) = f(y,x)$ appears natural since Q and P should be treated on equal footing. But this yields $y = x$ as a natural candidate for maximal information (examples 1–4). If in addition $f(1-x,y) = f(x,y)$ then also the complements $\mathbf{1}-Q$ and $\mathbf{1}-P$ are treated equivalently, and further solutions may lie on the line $y = 1-x$ (examples 1 and 4).

To conclude, there is again only a very limited connection between (non)commutativity and maximal information. In Ref. 4 it was pointed out that for the totally noncommutative spectral projections $E^Q(\mathbb{R}^+)$, $E^P(\mathbb{R}^+)$ one may have information arbitrarily close to the supremum without reaching it. For bounded X, Y, maximal information is achieved on the states satisfying $(E^Q(\mathbb{R}\setminus X) \wedge E^P(\mathbb{R}\setminus Y))\phi = \phi$ or $(E^Q(X) + E^P(Y))\phi = \|E^Q(X) + E^P(Y)\|\phi$; note that these $E^Q(X)$, $E^P(Y)$ are partially commutative. In general, both commutative and partially commutative projections admit absolutely maximal information in the sense of example 1, but this last example indicates that the measure of example 2 [without the symmetry $f(x,y) = f(1-x,y)$] is more suitable since it points more directly to a characterization of the degree of "reality" of $E^Q(X)$ and $E^P(Y)$: the larger the intervals X, Y are chosen, the larger the maximal probability sum $\|E^Q(X) + E^P(Y)\|$ will be.

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APPENDIX: PROOF OF THEOREM 1

Assume

$$f\mathscr{F}^{-1}[g\mathscr{F}(\phi)] = \mathscr{F}^{-1}[g\mathscr{F}(f\phi)] \qquad (*)$$

holds for all $\phi\in L^2(\mathbb{R},dq)$ and for some nonconstant $f,g\in L^\infty(\mathbb{R},dq)$. Fix f and let G_f denote the set of all $h\in L^\infty(\mathbb{R},dq)$ such that $(*)$ holds with g replaced by h for all $\phi\in L^2(\mathbb{R},dq)$. One sees that G_f is a nontrivial translation invariant subspace of $L^\infty(\mathbb{R},dq)$ which is closed in the weak*-topology of $L^\infty = (L^1)^*$. Let W be the weak*-closed subspace of $L^\infty(\mathbb{R},dq)$ spanned by g and its translates. Then $W\neq\{0\}$; hence W contains a character $V_\beta(x) = \exp(i\beta x)$ of $\mathbb{R}$, by Theorem 9 of Dunford and Schwartz.[11] By Theorem 16 of the same reference, W must contain a V_β with $\beta\neq 0$; in fact, if $V_0\equiv 1$ is the only character in W then $g = \text{const}\cdot V_0$; i.e., g is constant. Since $W\subset G_f$, we have $V_\beta\in G_f$ and hence

$$f\mathscr{F}^{-1}[V_\beta\mathscr{F}(\phi)] = \mathscr{F}^{-1}[V_\beta\mathscr{F}(f\phi)];$$

that is, $f\phi_\beta = f_\beta\phi_\beta$, for all $\phi\in L^2(\mathbb{R},dq)$, where $h_\beta(x) = h(x-\beta)$ for functions h. It follows that $f = f_\beta$ a.e.; i.e., β is a nonzero period of f. Conversely, if β is a period of f, then $V_\beta\in G_f$. Since f is measurable and nonconstant, f has a minimum period $\beta_0 > 0$. We can now reverse the roles of f and g; taking the Fourier transform of both sides of $(*)$ we see $(*)$ is equivalent to

$$g\mathscr{F}[f\mathscr{F}^{-1}(\hat\phi)] = \mathscr{F}[f\mathscr{F}^{-1}(g\hat\phi)],$$

where $\hat\phi = \mathscr{F}\phi$ is again a general element of $L^2(\mathbb{R},dq)$. We conclude that g must be periodic with minimum period $\alpha_0 > 0$. We may set $f = \Sigma c_n V_{n\alpha}$ where $\alpha = 2\pi/\beta_0$. This implies

$$\sum c_n\mathscr{F}^{-1}[g_{n\alpha}\mathscr{F}(V_{n\alpha}\phi)] = \mathscr{F}^{-1}\left[g\mathscr{F}\left[\sum c_n V_{n\alpha}\phi\right]\right];$$

or, taking $\mathscr{F}$,

$$\sum c_n g_{n\alpha}\mathscr{F}(V_{n\alpha}\phi) = g\sum c_n\mathscr{F}(V_{n\alpha}\phi), \quad \forall\phi\in L^2;$$

or

$$\sum c_n(g_{n\alpha} - g)\mathscr{F}(V_{n\alpha}\phi) = 0, \quad \forall\phi\in L^2;$$

or

$$\sum c_n(g_{n\alpha} - g)[\mathscr{F}(\phi)]_{n\alpha} = 0, \quad \forall\phi\in L^2.$$

Pick $m\in\mathbb{Z}$. For each $N\in\mathbb{Z}$, define $\phi_N\in L^2$ by

$$(\mathscr{F}\phi_N)(x) = \begin{cases} 1, & x\in[(N-m)\alpha,(N-m+1)\alpha), \\ 0, & \text{otherwise.}\end{cases}$$

Pick $y\in\mathbb{R}$. Then there is a unique N such that $y\in[N\alpha,(N+1)\alpha)$. Thus $[\mathscr{F}(\phi_N)]_{n\alpha}(y) = 0$ unless $m = n$. Hence

$$c_m(g_{m\alpha} - g)(y) = 0, \quad y\in[N\alpha,(N+1)\alpha), \text{ a.e.}$$

Since the choice N was arbitrary,

$$c_m (g_{m\alpha} - g)(y) = 0 \text{ a.e.}$$

Hence if $c_m \neq 0$, then $g_{m\alpha} = g$ a.e.; i.e., $m\alpha$ is a period for g. Since g has minimal period α_0 we must have the following.

If (g, f) is a solution pair for $(*)$ with minimal periods α_0, β_0, and for f written in the form

$$f = \sum c_n V_{n2\pi/\beta_0},$$

then

$c_n \neq 0 \Rightarrow \exists$ integer $z(n)$ such that

$$n2\pi/\beta_0 = z(n)\alpha_0.$$

Let $K = \{n \in \mathbb{Z} | c_n \neq 0\}$.

Let M be the subset of $\mathbb{Z}$ generated from the finite linear combinations of elements of K using integer coefficients. Here M is a closed subgroup of $\mathbb{Z}$, so there is an $n_0 \in \mathbb{Z}/\{0\}$ with $M = n_0\mathbb{Z}$. Thus every element n of k can be written $n = n_0 r$, some integer r. Then

$$f = \sum_r c_{n_0 r} V_{n_0 r 2\pi/\beta_0},$$

which has β_0/n_0 as a period. Since β_0 is the minimal period, we must have $n_0 = 1$. Now the equation

$$n2\pi/\beta_0 = z(n)\alpha_0,$$

$z(n)$ some integer, holds for all $n \in K$ and therefore for all $n \in M$. Thus there is an integer $z \neq 0$ such that

$$2\pi/\alpha_0\beta_0 = z.$$

Now we prove sufficiency. If either f or g is constant, $(*)$ holds trivially. Thus suppose f, g are periodic L^∞ functions with minimal periods β_0, α_0, respectively. Then one has for $\alpha = 2\pi/\beta_0$

$$V_{n\alpha}\mathcal{F}^{-1}[g\mathcal{F}(\phi)] = \mathcal{F}^{-1}[g_{n\alpha}\mathcal{F}(V_{n\alpha}\phi)]$$
$$= \mathcal{F}^{-1}[g\mathcal{F}(V_{n\alpha}\phi)]$$

whenever $n\alpha$ is a period of g. Multiplying by the c_n such that $f = \Sigma c_n V_{n\alpha}$ we obtain $(*)$ after invoking generalized α-periodicity.

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The problem of moments in the phase-space formulation of quantum mechanics

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Long ago, Moyal [Proc. Cambridge Philos. Soc. **45**, 99 (1949)] formulated a moment problem in the context of the Wigner–Weyl phase-space formulation of quantum mechanics. The problem amounts to giving necessary and sufficient conditions for a sequence of numbers to be moments of a Wigner function. In this paper, that problem is solved, and so is a truncated version of it.

I. INTRODUCTION

My purpose in writing this paper is to give necessary and sufficient conditions for the solution of a quantum mechanical moment problem first mentioned by Moyal in his seminal 1949 paper[1]: Given a sequence of numbers $m_{j,k}$, where j,k are the multi-indices

$$j=(j_1,\ldots,j_n)\,,\quad k=(k_1,\ldots,k_n)\,, \tag{1.1}$$

and n is some fixed positive integer, find necessary and sufficient conditions for there to be a Wigner distribution function $\rho(\mathbf{q},\mathbf{p})$, $\mathbf{q}=(q_1,\ldots,q_n)$, $\mathbf{p}=(p_1,\ldots,p_n)$, such that

$$m_{j,k}=\int\!\!\int \mathbf{p}^j\mathbf{q}^k\rho(\mathbf{q},\mathbf{p})\,d^nq\,d^np\,. \tag{1.2}$$

Here $\mathbf{p}^j$ and $\mathbf{q}^k$ stand for these quantities,

$$\mathbf{p}^j=p_1^{j_1}p_2^{j_2}\cdots p_n^{j_n}\,,\quad \mathbf{q}^k=q_1^{k_1}\cdots q_n^{k_n}\,. \tag{1.3}$$

In a recent paper,[2] O'Connell and I gave a set of *necessary* conditions for there to be a solution to this problem. While I will postpone any detailed discussion of that set, I do wish to make a few remarks about it.

The conditions in it amount to the non-negativity of a hierarchy of quadratic forms, where a given quadratic form has moments up to some fixed, even order for its coefficients. The simplest of these involves moments of order 2 or less, and its non-negativity is equivalent[2,3] to the position-momentum uncertainty relation. The conditions guaranteeing the non-negativity of other quadratic forms in the set place restrictions on the higher order moments analogous to those for the simplest case; these restrictions may thus be thought of as generalized uncertainty relations.

The set of necessary and sufficient conditions that I will give here includes the set that O'Connell and I derived in Ref. 2; the relationship between the two sets will be discussed in the last section of the paper. For now, I will simply describe the set that I will later show to be necessary and sufficient. This requires some notation and a word or two about the Wigner–Weyl phase-space formulation of quantum mechanics.

Let $z\equiv(\mathbf{q},\mathbf{p})$ denote a point in phase space Γ, which is $\mathbf{R}^n\times\mathbf{R}^n$ equipped with the symplectic form

$$\sigma(z,z')\equiv(2/\hbar)(\mathbf{p}\cdot\mathbf{q}'-\mathbf{q}\cdot\mathbf{p}') \tag{1.4}$$

and the measure

$$dz=dq_1\cdots dq_n\,dp_1\cdots dp_n\,. \tag{1.5}$$

Here $A(z)$, $B(z)$, $C(z)$, etc., will denote functions or tempered (Schwartz) distributions defined on phase space, and $\hat{A},\hat{B},\hat{C},\ldots$ will denote the operators associated with $A,B,C,\ldots$ via the Weyl transform.[4] The twisted product of A with B is

$$A\circ B(z)\equiv(\pi\hbar)^{-2n}\int\!\!\int A(z+z_1)B(z+z_2)\times e^{-i\sigma(z_1,z_2)}\,dz_1\,dz_2\,, \tag{1.6}$$

and is the Wigner transform[4] of $\hat{A}\hat{B}$. Finally, let

$$\langle A,B\rangle\equiv\int A(z)\,\overline{B(z)}\,dz\,. \tag{1.7}$$

I will bring in other notation as needed. For the most part I will use the same notation that I used in Ref. 4. (I also remark that Secs. I and II of Ref. 4 contain a brief review of the phase-space formulation of quantum mechanics.)

One can easily show[5] that if A and B are Schwartz functions—i.e., A,B are in $\mathcal{S}(\mathbf{R}^{2n})$, then $A\circ B$ is too. This allows us to define a notion of positivity on $\mathcal{S}'$, the set of tempered distributions. A tempered distribution F will be said to be $\hbar$ *positive* if

$$\langle F,A\circ\overline{A}\rangle\geqslant 0 \tag{1.8}$$

for every $A\in\mathcal{S}(\mathbf{R}^{2n})$. When this happens, I will write

$$F\overset{\hbar}{\geqslant}0\,. \tag{1.9}$$

In terms of operators, F being $\hbar$ positive means that

$$\langle F,A\circ\overline{A}\rangle=(2\pi\hbar)^n\,\mathrm{Tr}[\hat{F}\hat{A}\hat{A}^*]\geqslant 0\,. \tag{1.10}$$

From this it follows that $\hat{F}$ is a positive operator, and conversely.

Let $P(z)$ be any polynomial in $\mathbf{q},\mathbf{p}$, that is, let

$$P(z)=\sum_{j,k}c_{j,k}\,\mathbf{p}^j\mathbf{q}^k. \tag{1.11}$$

Next, define the "moment functional" μ via

$$\mu(P)=\sum_{j,k}c_{j,k}m_{j,k}\,. \tag{1.12}$$

If the $m_{j,k}$ are of the form (1.1), then it is easy to see that

$$\mu(P)=\int P(z)\rho(z)\,dz=\langle P,\rho\rangle\,. \tag{1.13}$$

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Since ρ is a Wigner function, it is the Wigner transform of a non-negative trace class operator; it thus has the form $\rho = G \circ G$. [Take $\widehat{G} = (\widehat{\rho})^{1/2}$.] From (1.13), one gets

$$\mu(P) = \langle P, G \circ G \rangle , \quad G = \overline{G} . \tag{1.14}$$

If $G \in \mathscr{S}(\mathbb{R}^{2n})$, all of the manipulations I have made are correct. Examining (1.14), I find that $\mu(P) \geqslant 0$ when P is $\hbar$ positive.

To anyone with experience in classical moment problems, it should not come as a surprise that μ being positive for $\hbar$-positive P is also a sufficient condition for a solution to the moment problem to exist. There is, however, a surprise in the kind of solution one gets. The main result of this paper is the following theorem.

Theorem 1.1: A necessary and sufficient condition for there to exist an (unnormalized) Wigner function $\rho = G \circ G$, with G real valued and in $\mathscr{S}$, for which (1.2) holds is that $\mu(P) \geqslant 0$ whenever P is an $\hbar$-positive polynomial in $\mathbf{q},\mathbf{p}$.

The surprise is, of course, that the Wigner function one gets to solve the moment problem (1.2) not only decays fast enough to support integrals of all powers of $\mathbf{p}$ and $\mathbf{q}$, but it is also infinitely smooth, a Schwartz function in fact. No such regularity arises in solutions to classical moment problems.

I will prove Theorem 1.1 in two major steps. The first step is to extend the moment functional μ to certain spaces that contain the polynomials and that consist of smooth functions which are themselves sufficiently nice that one may use them as symbols in the Weyl calculus; the extensions that I get will be positive on the $\hbar$-positive elements of these spaces. The next step, which is the harder of the two, is to come up with a representation for certain elements in the dual of the extension spaces; these elements are just the continuous linear functionals that are positive on the $\hbar$-positive functions in the extension spaces. Putting the two steps together gives the theorem.

The remainder of the paper is organized this way. In Sec. II, I will carry out the first step of the proof. That is, I will prove the existence of a continuous linear functional that is positive on the $\hbar$-positive elements of the extension spaces and that agrees with the moment functional μ when restricted to the polynomials. In Sec. III, I will carry out the second step in the proof. In addition, I will also solve a truncated version of the moment problem (1.2). Finally, in Sec. IV, I will discuss the connection between the set of necessary conditions that O'Connell and I gave in Ref. 2, and I will make a few concluding remarks.

II. EXTENSIONS OF THE MOMENT FUNCTIONAL

To carry out the "extension" step in the proof of the main result, I need an appropriate set of spaces to work with. It turns out that for the purposes I have in mind the symbol classes S_r introduced by Voros[5] will do nicely. These are defined this way: Let r be a fixed real number. The space S_r is defined as the set of all C^∞ functions A: $\Gamma \to \mathbb{C}$ that satisfy

$$\|A\|_{\alpha,r} \equiv \sup_{z \in \Gamma} \{ |\partial^\alpha A| (1 + |z|^2)^{(|\alpha| - r)/2} \} < \infty . \tag{2.1}$$

Here, $|z|^2 = \mathbf{q} \cdot \mathbf{q} + \mathbf{p} \cdot \mathbf{p}$, α is a multi-index, and ∂^α is the partial derivative corresponding to α. The $\| \ \|_{\alpha,r}$'s are seminorms on S_r, and they can be used in the usual way to construct a topology on S_r.

There are several reasons for using the S_r's. First, every polynomial of degree less than or, possibly, equal to r is contained in S_r. Second, the twisted product is defined for functions in these spaces. Indeed, if $A \in S_r$ and $B \in S_{r'}$, then[5] $A \circ B \in S_{r+r'}$. Third, functions in S_r are tempered distributions, for, when $|z|$ is large, they behave like polynomials. The set of functions in S_r that are also $\hbar$-positive tempered distributions is clearly a cone, which I will denote by S_r^+. Finally, the relationship between these spaces and the Weyl calculus is well understood.[5,6]

The space S_0 plays an important role here. One can show that there is a linear topological isomorphism between S_0 and S_r, and that this isomorphism associates the positive cones S_0^+ and S_r^+ with one another. In a bit, I will discuss this isomorphism. For now, I want to take a close look at the properties of S_0 itself. I will begin with this proposition.

Proposition 2.1: Let $A \in S_0$ and let A be real valued. There exists a continuous seminorm $\| \cdot \|_w$, defined on S_0, such that

$$\|A\|_w \pm A \in S_0^+ . \tag{2.2}$$

Proof: It is tedious, but quite straightforward, to show that the function

$$g_z(t) \equiv |t|^2/\hbar(1 + |z|^2) \tag{2.3}$$

defines what Hörmander terms a "slowly varying" metric on phase space (Ref. 6, Definition 18.4.1), and that the function

$$m_r(z) \equiv (1 + |z|^2)^{r/2} \tag{2.4}$$

is "g continuous" for g defined by (2.3). Thus Hörmander's symbol class (Ref. 6, Definition 18.4.2) $S(m_r, g_z)$ is well defined. Inspection of its definition shows that it is a Fréchet space identical with Voros's S_r. In particular, S_0 coincides with $S(1, g_z)$.

On the other hand, $S(1, g_z)$ satisfies the conditions necessary and sufficient for the L^2-operator norm of the Weyl transform of a symbol in $S(1, g_z)$ to provide a continuous seminorm on $S(1, g_z)$. [See Theorem 18.6.3, Ref. 6. Checking that this is the case is again tedious. The reader should also be aware of notational differences between Ref. 6 and this paper. To compare the two notational systems, set $h = 1$ here, and note that σ defined in (1.4) here is two times the σ Hörmander uses in Ref. 6.] Specifically, if $u(\mathbf{q}) \in L^2(\mathbb{R}^n)$, and if $A \in S(1, g_z)$, then

$$(\widehat{A}u)(\mathbf{q}) \equiv (2\pi\hbar)^{-n} \int e^{i\mathbf{p} \cdot (\mathbf{q} - \mathbf{q}')/\hbar} A\left(\frac{1}{2}(\mathbf{q} + \mathbf{q}'), \mathbf{p}\right) \times u(\mathbf{q}') d^n\mathbf{q}' \, d^n\mathbf{p} \tag{2.5}$$

is the Weyl transform of A. The norm $\|\widehat{A}\|_{\text{op}}$ is a continuous seminorm on the symbol space $S(1, g_z)$. I will denote this seminorm by

$$\|A\|_w \equiv \|\widehat{A}\|_{\text{op}} . \tag{2.6}$$

Let $F(z) \in \mathscr{S}(\Gamma)$, and recall that[5,7] the corresponding Weyl transform $\widehat{F}$ is a trace-class operator. Moreover,[7]

$$\int A(z)(F \circ \overline{F})(z) \, dz = (2\pi\hbar)^n \operatorname{tr}(\widehat{A}\widehat{F}\widehat{F}^*) . \tag{2.7}$$

If A is real, then $\widehat{A}$ is self-adjoint and satisfies

$$-\|\hat{A}\|_{\mathrm{op}}\cdot\hat{1}\leqslant\hat{A}\leqslant\|\hat{A}\|_{\mathrm{op}}\cdot\hat{1}\,. \tag{2.8}$$

This operator inequality is preserved if one premultiplies and postmultiplies by $\hat{F}^*$ and $\hat{F}$, respectively. Hence, one has that

$$-\|\hat{A}\|_{\mathrm{op}}\hat{F}^*\hat{F}\leqslant\hat{F}^*\hat{A}\hat{F}\leqslant\|\hat{A}\|_{\mathrm{op}}\hat{F}^*\hat{F}\,. \tag{2.9}$$

Using the fact that taking the trace in (2.9) will leave the sense of the inequalities unchanged and rewriting (2.9) in an obvious way, one gets

$$\mathrm{tr}(\hat{F}^*[\,\|\hat{A}\|_{\mathrm{op}}\cdot\hat{1}\pm\hat{A}\,]\hat{F})\geqslant 0\,. \tag{2.10}$$

From (2.6), (2.7), (2.10), and $\mathrm{tr}(\hat{R}\hat{S})=\mathrm{tr}(\hat{S}\hat{R})$, one finally arrives at this:

$$\int(\|A\|_w\pm A)F\circ\overline{F}\,dz\geqslant 0\,. \tag{2.11}$$

Since $S(1,g_z)$ and S_0 are the same Fréchet space, (2.11) holds for all real $A\in S_0$. From the definition of S_0^+, one sees that (2.11) implies (2.2).

For possible future reference, I want to draw off a corollary to the proof of Proposition 2.1.

Corollary 2.2: With g_z defined by (2.3) and $m_r(z)$ given by (2.4), Hörmander's symbol class $S(m_r,g_z)$ is the same Fréchet space as Voros's symbol class S_r.

What needs to be done next is to construct a mapping that makes S_0 and S_r topologically isomorphic and that associates S_0^+ with S_r^+. To do this, first let

$$H(z)\equiv\tfrac{1}{2}(\mathbf{q}\cdot\mathbf{q}+\mathbf{p}\cdot\mathbf{p})\,; \tag{2.12}$$

this is, of course, the classical Hamiltonian for n harmonic oscillators with all of the masses and frequencies taken to be 1. Next, define

$$H_r(z)\equiv\text{Wigner transform of }(\hat{H}^r). \tag{2.13}$$

(I will use a subscript and not a superscript because I want to avoid confusing powers relative to the twisted product with powers relative to ordinary multiplication.) These functions have the properties listed in the following.

Lemma 2.4: If r and t are real, and if H_r is given by (2.13), then H_r is real valued, belongs to S_{2r}, and satisfies

$$H_r\circ H_t=H_{r+t}\,. \tag{2.14}$$

Proof: Let $\beta>0$; define the operator

$$\hat{\Omega}_\beta\equiv\exp(-\beta\hat{H})\,. \tag{2.15}$$

Using standard functional analytic techniques, one can write

$$\hat{H}^{-r}=\frac{1}{\Gamma(r)}\int_0^\infty\beta^{r-1}\hat{\Omega}_\beta\,d\beta \tag{2.16}$$

for all $r>0$. Taking the Wigner transform of both sides and using the fact that the Wigner transform commutes with the integral in (2.16), one gets

$$H_{-r}(z)=\frac{1}{\Gamma(r)}\int_0^\infty\beta^{r-1}\Omega_\beta(z)\,d\beta\,, \tag{2.17}$$

where $\Omega_\beta(z)$, the Wigner transform of $\hat{\Omega}_\beta$, is given by

$$\Omega_\beta(z)=\mathrm{sech}^n(\hbar\beta/2)\times\exp(-[2H(z)/h\,]\tanh(\hbar\beta/2))\,. \tag{2.18}$$

The one-dimensional version of (2.18) is derived in Ref. 8. To get (2.18), one need only take products of the one-dimensional Wigner functions.

I now want to show that $H_{-r}\in S_{-2r}$. First, observe that

$$\partial^\alpha H_{-r}(z)=\sum_{|\gamma|\leqslant|\alpha|}z^\gamma g\int_0^\infty\beta^{r-1}\times\left[\tanh\left(\frac{\hbar\beta}{2}\right)\right]^{(|\gamma|+|\alpha|)/2}\Omega_\beta(z)\,d\beta\,; \tag{2.19}$$

here, c_γ depends on the multi-indices, α,γ, on $\hbar$, and nothing else.

The integral in (2.19) is easy to estimate for large values of $|z|$. Just break the interval of integration into $[0,1]$ and $[1,\infty)$. The part of the integral from $[1,\infty)$ decays like $\exp(-\mathrm{const}|z|^2)$. On the other hand, the part from $[0,1]$ satisfies

$$\int_0^1\beta^{r-1}\left[\tanh\left(\frac{\hbar\beta}{2}\right)\right]^{(|\gamma|+|\alpha|)/2}\Omega_\beta(z)\,d\beta\leqslant C\int_0^\infty\beta^{(2r+|\gamma|+|\alpha|)/2-1}\exp(-\beta H)\,d\beta\,,$$

and so it decays like $C|z|^{-2(2r+|\gamma|+|\alpha|)}$. The whole integral thus decays like the power estimate for the $[0,1]$ interval.

By what I have just found concerning the integral in (2.19), I get that for $|z|\to\infty$

$$|\partial^\alpha H_{-r}(z)|\leqslant C|z|^{-(2r+|\alpha|)}\,,$$

from which it immediately follows that $H_{-r}\in S_{-2r}$. To see that $H_r\in S_{2r}$ for $r\geqslant 0$, write r this way

$$r=k-(k-r)\,,$$

where k is any integer strictly larger than r. Because of the operator identity

$$\hat{H}^r=\hat{H}^r\cdot\hat{H}^{-(k-r)}\,,$$

one has that

$$H_r=H_k\circ H_{-(k-r)}\,.$$

Since $H=H_1$ is in S_2, because it is a polynomial of degree 2, $H_k=H\circ H\circ\cdots\circ H$ (k times) is in S_{2k}. The function $H_{-(k-r)}$ is, by the analysis above, in S_{2r-2k}. The twisted product of H_k and $H_{-(k-r)}$ is[5] then in $S_{2k+2r-2k}=S_{2r}$.

The formula (2.14) is the phase-space version of the corresponding operator identity. That $H_r(z)$ is real is obvious.

Lemma 2.4 is the key to constructing the isomorphism between S_0 and S_r that I mentioned earlier. To construct this, first observe[5] that the mapping $A\to A\circ H_{-r/4}$ takes S_t continuously into $S_{t-r/2}$, and that $B\to H_{-r/4}\circ B$ takes $S_{t-r/2}$ continuously into S_{t-r}. Thus

$$T_r(A)=H_{-r/4}\circ A\circ H_{-r/4} \tag{2.20}$$

defines a continuous, linear map from S_t to S_{t-r} for every $r,t\in\mathbb{R}$. Moreover, T_{-r} inverts T_r, for

$$\begin{aligned}T_{-r}(T_r(A))&=H_{r/4}\circ H_{-r/4}\circ A\circ H_{-r/4}\circ H_{r/4}\\&=H_0\circ A\circ H_0\\&=1\circ A\circ 1=A\,.\end{aligned}$$

Similarly, $T_r(T_{-r}(A))=A$. Since T_{-r} is a continuous linear map too, the mapping T_r sets up a topological isomorphism between the two Fréchet spaces S_t and S_{t-r}.

It is obvious that this isomorphism satisfies

$$\overline{T_r(A)} = T_r(\overline{A}) , \tag{2.21}$$

so that real-valued functions are associated with real-valued functions. What requires a little more work, but is more important here, is that S_t^+ and S_{t-r}^+ are associated via this isomorphism. To see that is so, one must show that $A \in S_t$ is $\hbar$ positive if and only if $T_r(A)$ is, too.

Let $A \overset{\hbar}{\geqslant} 0$. For every $B \in \mathscr{S}(\Gamma)$, one has that $H_{-r/4} \circ B$ is also in $\mathscr{S}(\Gamma)$, and that

$$\int A(z)(H_{-r/4} \circ B) \circ \overline{(H_{-r/4} \circ B)}\, dz \geqslant 0 . \tag{2.22}$$

Using the associativity of the twisted product and the identity

$$\int C \circ D\, dz = \int C(z) D(z)\, dz , \tag{2.23}$$

which applies under fairly general conditions, among which are included one of C,D being in $\mathscr{S}(\Gamma)$ while the other is in some S_r, one may justify these manipulations done on the right-hand side of (2.22),

$$\begin{aligned} \text{rhs of (2.22)} &= \int A \circ H_{-r/4} \circ B \circ \overline{B} \circ H_{-r/4}\, dz \\ &= \int H_{-r/4} \circ A \circ H_{-r/4} \circ B \circ \overline{B}\, dz \\ &= \int T_r(A) \circ B \circ \overline{B}\, dz \\ &= \langle T_r(A), B \circ \overline{B} \rangle . \end{aligned} \tag{2.24}$$

Hence, for all $B \in \mathscr{S}(\Gamma)$, (2.22) implies that

$$\langle T_r(A), B \circ \overline{B} \rangle \geqslant 0 , \tag{2.25}$$

and so $T_r(A) \overset{\hbar}{\geqslant} 0$. A similar manipulation justifies the reverse implication, and proves the following theorem.

Theorem 2.5: The mapping $T_r: S_t \to S_{t-r}$ defined in (2.20) is a continuous linear bijection for every $r,t \in \mathbb{R}$. The inverse of T_r is T_{-r}. Under T_r, $\hbar$-positive functions in S_t correspond to $\hbar$-positive functions in S_{t-r}, and real functions correspond to real functions.

To complete the "extension step," I need one last result.

Theorem 2.6: Let E be a self-adjoint subspace of S_r and suppose that $H_{r/2}(z) \in E$. If ϕ_0 is a linear functional that is defined on E, real on the real functions in E, and positive on $E \cap S_r^+$, then there exists a continuous linear functional ϕ that is defined on S_r, that is non-negative on S_r^+, and that agrees with ϕ_0 on E.

Proof: I begin by noting that $\hbar$-positive tempered distributions are real valued. The easiest way to see this is to observe that the symplectic Fourier transform of one is a tempered distribution of $\hbar$-positive type,[9] and that such a distribution satisfies a symmetry condition [Ref. 9, Proposition 3.1, (iii)] equivalent to the original distribution being real.

The point is that I may work entirely with the spaces $\mathrm{Re}(E)$ and $\mathrm{Re}(S_r)$, which compromise, respectively, the real-valued functions in E and S_r. Doing so allows me to use Krein's version[10] of the Hahn–Banach theorem to produce the extension ϕ.

Let $A \in \mathrm{Re}(S_r)$, and let

$$D \equiv H_{r/2} - A . \tag{2.26}$$

Note that for T_r defined by (2.20)

$$T_r(D) = 1 - T_r(A) , \tag{2.27}$$

and that

$$T_r(D) = 1 - \|T_r(A)\|_w + \|T_r(A)\|_w - T_r(A) ; \tag{2.28}$$

here, $\|\cdot\|_w$ is the continuous seminorm that was mentioned in Proposition 2.1. Composing $\|\cdot\|_w$ with T_r produces a continuous seminorm on S_r and, hence, on $\mathrm{Re}(S_r)$. The A's in $\mathrm{Re}(S_r)$ for which $\|\mathrm{Tr}(A)\|_w < 1$ clearly form a (real) neighbor of 0 in $\mathrm{Re}\, S_r$; call this neighborhood U. From Proposition 2.1, (2.28), and from the fact that positive constants belong to S_0^+, one sees that if $A \in U$, then $T_r(D)$ is in S_0^+. By Theorem 2.5, $T_r(D) \in S_0^+$ if and only if $D \in S_r^+$.

Since the D's in S_r^+ corresponding to the A's in U form a neighborhood of $H_{r/2}$, the conditions of Krein's theorem (Ref. 10, Theorem 2.6.3, p. 136) are fulfilled. Hence there exists a continuous, positive linear functional ϕ that extends ϕ_0 from $\mathrm{Re}(E)$ to $\mathrm{Re}(S_r)$. Simply by setting $\phi(f+ig) = \phi(f) + i\phi(g)$, for $f,g \in \mathrm{Re}(S_r)$, one gets the extension whose existence is asserted in the statement of the theorem.

I can now finish the extension step. In Theorem 2.6, let E be the space of polynomials in $\mathbf{q},\mathbf{p}$ of degree $2k$ or less. The functional ϕ_0 is replaced by the moment functional μ defined by (1.12). The conclusion of the theorem then gives the following corollary.

Corollary 2.7: For every integer $k \geqslant 0$, there exists a functional μ_k that is defined and continuous on S_{2k}, that is non-negative on S_{2k}^+, and that agrees with μ when restricted to the polynomials of degree $2k$ or less.

I close by remarking that μ_k will not usually be unique.

III. REPRESENTATIONS OF $\hbar$-POSITIVE LINEAR FUNCTIONALS

The next step in showing that the condition given in Theorem 1.1 is sufficient for there to be a solution of the moment problem that I discussed in the Introduction is to get representations for the functionals arising in Corollary 2.7. These functionals have two properties that enable me to get representations for them. First, they are in the topological dual of S_t, $t \geqslant 0$, and, second, they are non-negative when applied to $\hbar$-positive functions in S_t. I will call any functional that satisfies these two conditions an *$\hbar$-positive S functional.*

One can always restrict an $\hbar$-positive S functional ϕ to functions in Schwartz space, for $\mathscr{S}(\Gamma)$ is included in S_t for all real t. Moreover, because this inclusion is continuous,[5] $\phi|_{\mathscr{S}}$ is a continuous linear functional on $\mathscr{S}$; that is, $\phi|_{\mathscr{S}}$ is a tempered distribution. Finally, $\phi|_{\mathscr{S}}$ is an *$\hbar$-positive* tempered distribution because it is non-negative on S_t^+ and, for every $F \in \mathscr{S}$, $F \circ \overline{F} \in \mathscr{S} \cap S_t^+$. In summary, I have obtained the following lemma.

Lemma 3.1: Every $\hbar$-positive S functional ϕ, when restricted to $\mathscr{S}$, is an $\hbar$-positive tempered distribution.

The restricted $\hbar$-positive S functional ϕ being a tempered distribution implies that its symplectic Fourier transform $\tilde{\phi}$ is, too. Here $\tilde{\phi}$ is defined in the usual way,[11,12] via transpose. The version of the symplectic Fourier transform used here is the same as the one in Ref. 4,

$$\tilde{A}(a) = (\pi\hbar)^{-n} \int A(z) e^{i\sigma(a,z)}\, dz\,, \tag{3.1}$$

where $a \equiv (\mathbf{u},\mathbf{v}) = (u_1,\ldots,u_n,v_1,\ldots,v_n)$. As is the case with the ordinary Fourier transform, the symplectic Fourier transform takes Schwartz functions to Schwartz functions, and tempered distributions to tempered distributions.

The $\hbar$ positivity of ϕ is reflected in $\tilde{\phi}$'s being of $\hbar$-positive type.[9] This is easy to show. First, recall that[13]

$$\widetilde{A \circ B} = \tilde{A} \times \tilde{B}\,, \tag{3.2}$$

where $\tilde{A} \times \tilde{B}$ is the twisted convolution of $\tilde{A}$ with $\tilde{B}$ and is given by

$$\tilde{A} \times \tilde{B}(a) = (\pi\hbar)^{-n} \int \tilde{A}(b)\tilde{B}(a-b) e^{i\sigma(b,a)}\, db\,. \tag{3.3}$$

Second, note that

$$\tilde{F}^{\dagger}(a) \equiv \bar{\tilde{F}}(-a) = \tilde{\bar{F}}(a)\,. \tag{3.4}$$

Finally, observe that

$$\tilde{\phi}(\tilde{F} \times \tilde{F}^{\dagger}) = \tilde{\phi}(\widetilde{F \circ \bar{F}}) = \phi(F \circ \bar{F}) \geqslant 0\,, \tag{3.5}$$

the last inequality on the right-hand side being a consequence of ϕ's $\hbar$ positivity.

So far, everything I have said would be true if ϕ were merely an $\hbar$-positive distribution rather than an $\hbar$-positive S functional. The main consequence of ϕ's being an $\hbar$-positive S functional is that, for $A \in S_0$,

$$\phi(\|A\|_w \pm A) \geqslant 0\,, \tag{3.6}$$

because, by Proposition 2.1, $\|A\|_w \pm A \in S_0^{+}$. Clearly, (3.6) implies that if also $A \in \mathcal{S}(\Gamma)$,

$$|\tilde{\phi}(\tilde{A})| = |\phi(A)| \leqslant \phi(1)\|A\|_w\,. \tag{3.7}$$

Using a proof somewhat similar to that of Proposition 2.1, one may show that

$$\|A\|_w \leqslant 2^n \|\tilde{A}\|_{L^1}\,, \tag{3.8}$$

and so

$$|\tilde{\phi}(\tilde{A})| \leqslant 2^n \phi(1) \|\tilde{A}\|_{L^1}\,. \tag{3.9}$$

Finally, one may take limits in (3.9) to get that $\tilde{\phi}$ is a continuous, linear functional on L^1. Because L^{∞} is the dual of L^1, there is some function $\tilde{\Phi} \in L^{\infty}$ for which

$$\tilde{\phi}(\tilde{A}) = \int \tilde{\Phi}(a)\tilde{A}(a)\, da\,. \tag{3.10}$$

Since $\tilde{\phi}$ is an $\hbar$-positive type tempered distribution that is given by an L^{∞} function, one has, by Theorem 3.1 and Theorem 5.2 of Ref. 9, that there exists a function $\tilde{G}$ such that $\tilde{G} \in L^2$, $\tilde{G}^{\dagger} = \tilde{G}$, and

$$\tilde{\Phi}(a) = \tilde{G} \times \tilde{G}^{\dagger}(a)\,. \tag{3.11}$$

Unwinding the symplectic Fourier transforms then proves the following theorem.

Theorem 3.2: If ϕ is an $\hbar$-positive S functional, then there exists a real $G \in L^2$ such that

$$\phi(A) = \int A(z) G \circ G(z)\, dz \tag{3.12}$$

for all $A \in \mathcal{S}(\Gamma)$.

I remark that examination of the proof of Theorem 3.2 shows that one also has the following result.

Corollary 3.3: If ϕ is an $\hbar$-positive tempered distribution that satisfies

$$|\phi(A)| \leqslant c\|\tilde{A}\|_{L^1}\,, \tag{3.13}$$

then, for all $A \in \mathcal{S}(\Gamma)$, ϕ has the form (3.12).

In a certain sense, Theorem 3.2 gives the representation that I need. The difficulty is that it does not contain enough information about G to be useful in getting sufficiency in Theorem 1.1. To overcome this difficulty, I will take a close look at the properties of G when the ϕ that gives rise to it is in S_t^{*}, the topological dual of S_t. Doing this requires looking at the H_t's introduced in Sec. II.

The operator $\hat{H}$ corresponding to $H(z)$, which is given by (2.12), is the Hamiltonian for a system of n harmonic oscillators. The spectrum of $\hat{H}$ consists of discrete positive eigenvalues, each being of finite multiplicity; ∞ is the only limit point. The eigenvectors ψ_k, $k = 0,1,2,\ldots$, may be chosen to be real-valued functions. Of course, they are Schwartz functions that comprise an orthonormal basis for $L^2(\mathbb{R}^n)$. I will label the eigenvalue corresponding to ψ_k by λ_k. (Since some eigenvalues are degenerate, one can have $\lambda_k = \lambda_{k'}$ for $k \neq k'$. This can happen for only a finite number of indices, however.)

Using the ψ_k's, one may form Schwartz functions that comprise an orthonormal basis for $L^2(\Gamma)$. To do this, define[14]

$$\hat{B}_{j,k} \equiv \psi_j \otimes \psi_k\,; \tag{3.14}$$

these form an orthonormal basis for the space of Hilbert–Schmidt operators. By virtue of the unitary equivalence[15] between the space of Hilbert–Schmidt operators and $L^2(\Gamma)$, the set $\{B_{j,k}\}$, where $B_{j,k}$ is the Wigner transform of $\hat{B}_{j,k}$, is an orthogonal basis for $L^2(\Gamma)$. One may make it orthonormal by dividing each $B_{j,k}$ by $(2\pi\hbar)^{n/2}$. That each $B_{j,k}$ is a Schwartz function follows from the ψ_j's being products of Gaussians and Hermite polynomials, together with a standard argument from harmonic analysis.

My reason for introducing the $B_{j,k}$'s is that they diagonalize three different operators. First, define, for $A \in \mathcal{S}(\Gamma)$,

$$\begin{aligned} K_+(A) &= H \circ A\,, \\ K_-(A) &= A \circ H\,, \\ K_0(A) &= \tfrac{1}{2}(H \circ A + A \circ H) = \tfrac{1}{2}(K_+ + K_-)(A)\,. \end{aligned} \tag{3.15}$$

Each of these operators has $B_{j,k}$ as an eigenvector; indeed, this is obvious from the following lemma.

Lemma 3.4: Let K_+, K_-, and K_0 be defined by (3.15). Each operator is essentially self-adjoint on $\mathcal{S}(\Gamma)$, non-negative, and satisfies the following:

$$\begin{aligned} &K_+(B_{j,k}) = \lambda_j B_{j,k}\,, \quad K_-(B_{j,k}) = \lambda_k B_{j,k}\,, \\ &K_0(B_{j,k}) = [(\lambda_j + \lambda_k)/2] B_{j,k}\,. \end{aligned} \tag{3.16}$$

Proof: All three cases are so similar that only one of them needs doing. I will work with the statements involving K_+, and I will begin by getting (3.16).

Using the definition of $B_{j,k}$, note that these hold:

$$\begin{aligned}\widehat{K_+(B_{j,k})} &= \hat{H}\hat{B}_{j,k} \\ &= \hat{H}(\psi_j \otimes \psi_k) \\ &= (\hat{H}\psi_j) \otimes \psi_k \\ &= \lambda_j \psi_j \otimes \psi_k = \lambda_k \hat{B}_{j,k} .\end{aligned}$$

Taking Wigner transforms gives (3.16) for K_+.

Next I will show that K_+ is Hermitian on $\mathscr{S}(\Gamma)$. If A and B are Schwartz functions, then one has the following:

$$\begin{aligned}\langle K_+(A), B\rangle &= \int H\circ A\, \overline{B}\, dz \\ &= \int A\circ\overline{B}\circ H\, dz \\ &= \int A\circ \overline{(H\circ B)}\, dz \\ &= \langle A, K_+(B)\rangle .\end{aligned}$$

I remark that if one sets $A = B$ in the equations above, one also has that

$$\langle K_+(A), A\rangle = \int HA\circ\overline{A}\, dz ,$$

which is non-negative because H is $\hbar$ positive. Thus K_+ is non-negative.

All that remains is essential self-adjointness. This amounts to showing that $\pm i$ are *not* eigenvalues of K_+^* (Ref. 16, pp. 98 and 99). If they were, one would have $A\in L^2(\Gamma)$ for which $(K_+^* \pm i)A_\pm = 0$. Thus

$$0 = \langle B_{j,k}, (K_+^* \pm i)A_\pm \rangle ,$$

and so

$$0 = \langle (K_+ \pm i)B_{j,k}, A_\pm \rangle .$$

Since $K_+(B_{j,k}) = \lambda_j B_{j,k}$, and since λ_j is real, this equation implies that $\langle B_{j,k}, A_\pm\rangle = 0$. Thus $\{B_{j,k}\}$ being an orthogonal basis then implies that $A_\pm = 0$. Consequently, K_+ is essentially self-adjoint.

The essential self-adjointness of these operators is important, for coupling it with (3.16) and the orthogonality of the basis $\{B_{j,k}\}$ yields the spectral resolution for all three operators. One may then use that spectral resolution to prove the next lemma.

Lemma 3.5: Let K_+ and K_- be defined by (3.15), let H_t be given by (3.13), and let Ω_β be given by (2.18). If A is a Schwartz function, then these hold for any real t and all $\beta > 0$:

$$\begin{aligned}&K_+^t(A) = H_t\circ A , \quad K_-^t(A) = A\circ H_t , \\ &\exp(-\beta K_+)A = \Omega_\beta\circ A , \\ &\exp(-\beta K_-)A = A\circ\Omega_\beta .\end{aligned} \tag{3.17}$$

Proof: For each equation, simply compute the inner product of both sides with each of the $B_{j,k}$, and observe that the results from the two sides are equal. This is sufficient to establish the equations in an L^2 sense, which is all I really need.

The operators K_+, K_-, and K_0 all have fairly simple expressions in terms of partial differential operators. For example, if $A\in\mathscr{S}(\Gamma)$, then $K_+(A) = H\circ A$. But $H\circ A$ may be directly computed using Voros's Theorem 2.4.1,[5]

$$\begin{aligned}H\circ A = \sum_{j=1}^n \Bigg\{ &\frac{1}{2}(p_j^2 + q_j^2)A + \frac{i\hbar}{2}\left(q_j\frac{\partial A}{\partial p_j} - p_j\frac{\partial A}{\partial p_j}\right) \\ &- \frac{\hbar^2}{8}\left(\frac{\partial^2 A}{\partial p_j^2} + \frac{\partial^2 A}{\partial q_j^2}\right)\Bigg\} .\end{aligned} \tag{3.18}$$

Using $A\circ H = \overline{H\circ\overline{A}}$, one also has

$$\begin{aligned}A\circ H = \sum_{j=1}^n \Bigg\{ &\frac{1}{2}(p_j^2 + q_j^2)A - \frac{i\hbar}{2}\left(q_j\frac{\partial A}{\partial p_j} - p_j\frac{\partial A}{\partial q_j}\right) \\ &- \frac{\hbar^2}{8}\left(\frac{\partial^2 A}{\partial p_j^2} + \frac{\partial^2 A}{\partial q_j^2}\right)\Bigg\} .\end{aligned} \tag{3.19}$$

Putting these in vector notation and using them to compute $\frac{1}{2}(A\circ H + H\circ A)$, one easily gets these expressions for K_+, K_-, and K_0,

$$\begin{aligned}K_\pm &= \frac{1}{2}|z|^2 \pm \frac{i\hbar}{2}\left(\mathbf{q}\cdot\frac{\partial}{\partial\mathbf{p}} - \mathbf{p}\cdot\frac{\partial}{\partial\mathbf{q}}\right) \\ &\quad - (\hbar^2/8)(\Delta_p + \Delta_q) ,\end{aligned} \tag{3.20}$$

$$K_0 = \tfrac{1}{2}|z|^2 - (\hbar^2/8)(\Delta_p + \Delta_q) .$$

Observe that K_0 is the quantum mechanical Hamiltonian for $2n$ decoupled harmonic oscillators. Here $K_\pm$ are both perturbations of K_0 by an angular momentum term. While points in the spectrum of $K_\pm$ have infinite multiplicity, points in the spectrum of K_0 have only finite multiplicity. Also, for every $t > 0$, the domain of K_0^t is a compact subset of $L^2(\Gamma)$.

With these comments about K_0 in mind, the significance of my characterization of the G that appears in (3.12) will be apparent.

Theorem 3.6: Let ϕ be an $\hbar$-positive S functional in the topological dual of S_{2t}, $t\geqslant 0$. If G is as in (3.12), then G belongs to the domain of $K_0^{t/2}$.

Proof: Since $H_t\in S_{2t}$, and Ω_β, which is given in (2.18), belongs to $\mathscr{S}(\Gamma)$, $H_t\circ\Omega_\beta$ also belongs to $\mathscr{S}(\Gamma)$.[5] By Theorem 3.2, one has

$$\phi(H_t\circ\Omega_\beta) = \int (H_t\circ\Omega_\beta)(z) G\circ G(z)\, dz . \tag{3.21}$$

Using the associativity of the twisted product and (2.23), one may put (3.21) in this form,

$$\phi(H_t\circ\Omega_\beta) = \langle H_t\circ\Omega_\beta\circ G, G\rangle . \tag{3.22}$$

I want to get a bound for $\phi(H_t\circ\Omega_\beta)$, a bound that is independent of β. To do this, first note that one has the operator inequality

$$\hat{H}^t - \hat{H}^t e^{-\beta\hat{H}} \geqslant 0 .$$

In terms of phase-space functions, this inequality becomes

$$H_t - H_t\circ\Omega_\beta \overset{\hbar}{\geqslant} 0 . \tag{3.23}$$

Hence $H_t - H_t\circ\Omega_\beta \in S_{2t}^+$. The $\hbar$ positivity of ϕ then implies that

$$\phi(H_t\circ\Omega_\beta) \leqslant \phi(H_t) , \tag{3.24}$$

which is the bound I was looking for.

By approximating G with Schwartz functions, one may use Lemma 3.5 to show that

$$H_t \circ \Omega_\beta \circ G = K_+^t \, e^{-K_+ \beta}(G) , \tag{3.25}$$

which holds in an L^2 sense. Expand G in the basis $\{B_{j,k}\}$,

$$\begin{aligned} G &= \sum_{j,k} \gamma_{j,k} \, B_{j,k} , \\ \gamma_{j,k} &= (2\pi\hbar)^{-n} \langle G, B_{j,k} \rangle . \end{aligned} \tag{3.26}$$

Using (3.25), (3.26), and (3.16), one sees that

$$\langle H_t \circ \Omega_\beta \circ G, G \rangle = (2\pi\hbar)^n \left(\sum_{j,k} \lambda_j^t \, e^{-\beta\lambda_j} |\gamma_{j,k}|^2 \right) . \tag{3.27}$$

Putting (3.27) together with (3.22) and (3.24), one arrives at the inequality

$$\sum_{j,k} \lambda_j^t \, e^{-\beta\lambda_j} |\gamma_{j,k}|^2 \leqslant (2\pi\hbar)^{-n} \phi(H_t) , \tag{3.28}$$

from which it immediately follows that

$$\sum_{j,k} \lambda_j^t |\gamma_{j,k}|^2 \leqslant (2\pi\hbar)^{-n} \phi(H_t) . \tag{3.29}$$

The inequality in (3.29) is precisely the condition required for G to be in the domain of $K_+^{t/2}$; indeed,

$$\| K_+^{t/2} G \|^2 = (2\pi\hbar)^n \left(\sum_{j,k} \lambda_j^t |\gamma_{j,k}|^2 \right) \leqslant \phi(H_t) . \tag{3.30}$$

So far, I have not used the fact the G is a real-valued function. This reality is reflected in the $\gamma_{j,k}$'s obeying

$$\bar{\gamma}_{j,k} = \gamma_{k,j} . \tag{3.31}$$

To see this, first take the complex conjugate of both sides in the equation for $\gamma_{j,k}$,

$$\bar{\gamma}_{j,k} = (2\pi\hbar)^{-n} \langle \bar{G}, \bar{B}_{j,k} \rangle . \tag{3.32}$$

Since G is real, $G = \bar{G}$. On the other hand,

$$\bar{B}_{j,k} = \hat{B}^*_{j,k} = (\psi_j \otimes \psi_k)^* , \tag{3.33}$$

from (3.14). But $(x \otimes y)^* = y \otimes x$,[14] so

$$\hat{B}^*_{j,k} = \psi_k \otimes \psi_j = \hat{B}_{k,j} . \tag{3.34}$$

From (3.33) and (3.34), one gets that

$$\overline{B_{j,k}} = B_{k,j} . \tag{3.35}$$

Hence (3.32) may be written

$$\bar{\gamma}_{j,k} = (2\pi\hbar)^{-n} \langle G, B_{k,j} \rangle , \tag{3.36}$$

from which (3.31) follows directly.

In the sum in (3.30), use $|\gamma_{j,k}| = |\bar{\gamma}_{j,k}| = |\gamma_{k,j}|$, and then interchange summation indices; this yields

$$\| K_+^{t/2} G \|^2 = (2\pi\hbar)^n \left(\sum_{j,k} \lambda_k^t |\gamma_{j,k}|^2 \right) \leqslant \phi(H_t) . \tag{3.37}$$

As before, this implies that G is in the domain of $K_-^{t/2}$, and that

$$\| K_+^{t/2} G \|^2 = \| K_-^{k/2} G \|^2 \leqslant \phi(H_t) . \tag{3.38}$$

The final step in the proof begins with the observation that if $a > 0$, $b > 0$, and $t > 0$, then

$$2^{-t-1}(a^t + b^t) \leqslant ((a+b)/2)^t \leqslant a^t + b^t . \tag{3.39}$$

Using (3.30), (3.37), and the right half of (3.39), one gets

$$(2\pi\hbar)^n \left(\sum_{j,k} \left(\frac{\lambda_j + \lambda_k}{2} \right)^t |\gamma_{j,k}|^2 \right) \leqslant 2\phi(H_t) . \tag{3.40}$$

From (3.40), (3.16), and the argument that I just used, one again sees that G belongs to the domain of $K_0^{t/2}$. Indeed, putting together the various inequalities that one can arrive at from (3.30) and (3.38)–(3.40), I find that

$$2^{-t} \| K_+^{t/2} G \|^2 \leqslant \| K_0^{t/2} G \|^2 \leqslant 2 \| K_+^{t/2} G \|^2 \leqslant 2\phi(H_t) . \tag{3.41}$$

In the course of proving the theorem, I have actually proved somewhat more than what was stated. I shall summarize these additional results below.

Corollary 3.7: With the notation and assumptions of Theorem 3.6, one has that G belongs to the domains of both $K_+^{t/2}$ and $K_-^{t/2}$.

This corollary will be a help in answering the following natural and important question: To what extent does G determine the functional ϕ? Although I did not mention it in Theorem 3.2, G is unique if one also requires that it be $\hbar$ positive, so, in a sense, ϕ uniquely determines G. The converse is almost true. It will turn out that if $\phi \in S_t^*$, then for all $A \in S_r$, $r < t$, $\phi(A)$ is uniquely determined by G. To prove this, I need this lemma.

Lemma 3.8: If $A \in S_t$, then for every $\beta > 0$, both $A \circ \Omega_\beta$ and $\Omega_\beta \circ A$ belong to $\mathscr{S}(\Gamma)$. Moreover, for every $\epsilon > 0$, both $A \circ \Omega_\beta$ and $\Omega_\beta \circ A$ converge, in the topology of $S_{t+\epsilon}$, to A as $\beta \to 0^+$.

Proof: The first statement follows from Voros's theorem 2.4.1.[5] To get the rest of the lemma, all I really need to show is that, in S_ϵ, $\Omega_\beta \to 1$ as $\beta \to 0^+$; the statement about the convergence of $A \circ \Omega_\beta$ and $\Omega_\beta \circ A$ is simply a consequence of $\Omega_\beta \to 1$ and the continuity of the twisted product for Voros's symbols.[5]

To show that $\Omega_\beta \to 1$ in S_ϵ, note that

$$\begin{aligned} &\partial^\alpha (\Omega_\beta - 1)(z) \\ &\quad = \sum_{|\gamma| \leqslant |\alpha|} c_\gamma \, z^\gamma \left[\tanh\left(\frac{\hbar\beta}{2} \right) \right]^{(|\gamma| + |\alpha|)/2} \Omega_\beta(z) , \end{aligned} \tag{3.42}$$

where c_γ depends on α, γ, $\hbar$, but *not* on z or β. (Here, γ is a multi-index; it is not related to the $\gamma_{j,k}$'s used earlier.) For $R > 0$, one may use (3.42) together with a little calculus to show that

$$\begin{aligned} &\sup_{|z| > R} |\partial^\alpha (\Omega_\beta - 1)(z) (1 + |z|^2)^{(|\alpha| - \epsilon)/2}| \\ &\quad \leqslant C(1 + R^2)^{-\epsilon/2} , \end{aligned} \tag{3.43}$$

where C is independent of R, β. Since, on compact subsets of Γ, $\partial^\alpha(\Omega_\beta - 1)$ converges uniformly to 0 as $\beta \to 0^+$, one has, from (3.43) and (2.1), that

$$\limsup_{\beta \to 0^+} \| \Omega_\beta - 1 \|_{\alpha,\epsilon} \leqslant C(1 + R^2)^{-\epsilon/2} . \tag{3.44}$$

Letting $R \to \infty$ then yields that $\| \Omega_\beta - 1 \|_{\alpha,\epsilon} \to 0$ for all multi-indices α, and so $\Omega_\beta \to 1$ in S_ϵ.

I can now prove the assertion that I made just prior to Lemma 3.8.

Proposition 3.9: Let $t \geqslant 0$, $r < 2t$, and suppose that the $\hbar$-positive S functional ϕ is in S_{2t}^*. If $A \in S_r$, then

$$\phi(A) = \lim_{\beta\to 0^+}\left(\int A\circ\Omega_\beta G\circ G\, dz\right). \tag{3.45}$$

Proof: By Lemma 3.8, $A\circ\Omega_\beta\in\mathcal{S}(\Gamma)$, and so (3.12) holds:

$$\phi(A\circ\Omega_\beta) = \int (A\circ\Omega_\beta)(z) G\circ G(z)\, dz\,. \tag{3.46}$$

Again by Lemma 3.8, $A\circ\Omega_\beta\to A$ in $S_{r+\epsilon}$ for all $\epsilon>0$. With $\epsilon = 2t - r$, one sees that $A\circ\Omega_\beta\to A$ in S_{2t}:

$$\lim_{\beta\to 0^+}\phi(A\circ\Omega_\beta) = \phi(A)\,. \tag{3.47}$$

Combining (3.46) and (3.47) yields (3.45).

Thus G uniquely determines ϕ on all of the S_r's with $r<2t$. Sad to say, G does not always determine ϕ on S_{2t}. The reason for this is related to the existence of certain functionals in the dual of the space of bounded operators on a Hilbert space. These functionals have the property that they are non-negative, and they annihilate every compact operator; that is, they "live" on the Calkin algebra.[17] Although I do not need to deal with them here, I will say a bit more about their effects later.

What I *do* need is to get an explicit formula for ϕ in terms of G when ϕ is restricted to S_r. Let $A\in\mathcal{S}(\Gamma)$. For the present, also suppose that $G\in\mathcal{S}(\Gamma)$. Under these assumptions, one has that

$$\begin{aligned}
&\int A(z)G\circ G(z)dz \\
&\quad = \int H_{t/2}\circ H_{-t/2}\circ A\circ H_{-t/2}\circ H_{t/2}\circ G\circ G\, dz \\
&\quad = \int H_{t/2}\circ T_{-2t}(A)\circ H_{t/2}\circ G\circ G\, dz \\
&\quad = \int T_{-2t}(A)\circ H_{t/2}\circ G\circ \overline{(H_{t/2}\circ G)}\, dz \\
&\quad = \int T_{-2t}(A)\circ K_+^{t/2}G(z)\,\overline{K_+^{t/2}G(z)}\, dz \\
&\quad = \langle T_{-2t}(A)\circ K_+^{t/2}G, K_+^{t/2}G\rangle\,.
\end{aligned} \tag{3.48}$$

Here $T_{-2t}(A)$ is defined by (2.20).

If G is merely in the domain of $K_+^{t/2}$, one can show that (3.48) still holds. To do this, approximate G by a truncated version of (3.26),

$$G_N \equiv \sum_{j<N,\ k<N}\gamma_{j,k}B_{j,k}\,. \tag{3.49}$$

Here G_N is a finite sum of functions in $\mathcal{S}$, so it itself is in $\mathcal{S}$. Note that both G_N and $K_+^{t/2}G_N$ converge in L^2 to G and $K_+^{t/2}G$, respectively. Since the twisted product is L^2 continuous,[15] taking limits in

$$\int AG_N\circ G_N\, dz = \langle T_{-2t}(A)\circ K_+^{t/2}(G_N), K_+^{t/2}(G_N)\rangle$$

then yields (3.48) for any real G in the domain of $K_+^{t/2}$, and for any A in $\mathcal{S}$.

To get a formula for any A in S_r, $r<2t$, just write (3.48) in terms of a trace; that is, recast (3.48) as

$$\begin{aligned}
\int A(z)G\circ G\, dz &= \phi(A) = (2\pi\hbar)^n \operatorname{Tr}[\widehat{T_{-2t}(A)}\,\widehat{K_+^{t/2}(G)}\,\widehat{K_+^{t/2}(G)}^*]. \\
&\qquad\qquad (3.50)
\end{aligned}$$

In (3.50), replace A by $A\circ\Omega_\beta$, and use (3.45), Lemma 3.8, Theorem 2.5, and (1.7) to get the following proposition.

Proposition 3.10: Let ϕ, r, t, be as in Proposition 3.9. If $A\in S_r$ and G is as in (3.12), then

$$\phi(A) = (2\pi\hbar)^n \operatorname{Tr}[\widehat{T_{-2t}(A)}\,\widehat{K_+^{t/2}(G)}\,\widehat{K_+^{t/2}(G)}^*]\,. \tag{3.51}$$

One should note that the right-hand side of (3.51) defines an $\hbar$-positive S functional on S_{2t}; I will denote this functional by ϕ_G. Equation (3.51) shows that $\phi=\phi_G$ on all of the S_r's, $r<2t$. On the other hand, it is quite possible for $\phi\neq\phi_G$ on S_{2t}. For example, if ϕ_c is a positive, continuous linear functional on the bounded operators on $L^2(\mathbb{R}^n)$, and if ϕ_c annihilates the compact operators, then

$$\phi(A) = \phi_c(\widehat{T_{-2t}(A)}) + \phi_G(A) \tag{3.52}$$

defines an $\hbar$-positive S functional that differs from ϕ_G only for functions in S_{2t}; on S_r, $r<2t$, they agree because $\widehat{T_{-2t}(A)}$ turns out to be compact for $A\in S_r$.[5]

Suppose that one has another $\hbar$-positive S functional ϕ' and that it satisfies the same conditions that I imposed on ϕ in Proposition 3.9. In addition, let G' be the functional that corresponds to ϕ' via (3.12). Using (3.51) and few facts[14] concerning the relationships among $\|\cdot\|_{\mathrm{op}}$, $\operatorname{Tr}(\cdot)$, and Hilbert–Schmidt norm $\|\cdot\|_{\mathrm{HS}}$, one can show that for all $A\in S_r$, $r<2t$, one has this inequality,

$$\begin{aligned}
&|\phi(A)-\phi'(A)| \\
&\quad\leqslant (2\pi\hbar)^n \|\widehat{T_{-2t}(A)}\|_{\mathrm{op}}\,[\,\widehat{\|K_+^{t/2}G\|}_{\mathrm{HS}} \\
&\qquad + \|\widehat{K_+^{t/2}G'}\|_{\mathrm{HS}}\,]\{\widehat{\|K_+^{t/2}(G-G')\|}_{\mathrm{HS}}\}\,.
\end{aligned} \tag{3.53}$$

Putting this in terms of phase-space quantities, i.e., $\|\cdot\|_{\mathrm{op}} = \|\cdot\|_w$, $(2\pi\hbar)^{n/2}\|\cdot\|_{\mathrm{HS}} = \|\cdot\|_{L^2}$, one has the following result.

Corollary 3.11: Let $t\geqslant 0$, $r<2t$, and suppose that both ϕ and ϕ' are $\hbar$-positive S functionals in S_{2t}^*, and that G and G' are the corresponding functions given in (3.12). If $A\in S_r$, then

$$\begin{aligned}
|\phi(A)-\phi'(A)| &\leqslant \|\widehat{T_{-2t}(A)}\|_w\,[\,\widehat{\|K_+^{t/2}G\|}_{L^2} \\
&\qquad + \|\widehat{K_+^{t/2}G'}\|_{L^2}\,]\,\widehat{\|K_+^{t/2}(G-G')\|}_{L^2}\,.
\end{aligned} \tag{3.54}$$

What about the moment problem itself? I am now ready to finish proving that the conditions given in Sec. I are sufficient.

Proof of Theorem 1.1: In Sec. I, I showed that a necessary condition for the moment problem (1.2) to have a solution is that the moment functional be non-negative on every $\hbar$-positive polynomial P. If I assume, on the other hand, that $\mu(P)\geqslant 0$ for each $\hbar$-positive P, then by Corollary 2.7 there exists an $\hbar$-positive S functional $\mu_k\in S_{2k}^*$ such that $\mu_k(P)=\mu(P)$, when the degree of P is $2k$ or less. Theorems 3.2 and 3.6 imply that for each μ_k there exists a function G_k such that G_k belongs to the domain of $K_0^{k/2}$. Since, for $j=0,\ldots,[k/2]$, $S_{4j}^*\supseteq S_{2k}^*$, G_k belongs to the domain of K_0^j (which is obvious anyway), and, from (3.41), satisfies

$$\|K_0^j G_k\|_{L^2}^2 \leqslant 2\mu_k(H_{2j}) .$$

Because H_j is a polynomial of degree $4j \leqslant 2k$, this inequality may be rewritten as

$$\|K_0^j G_k\|_{L^2}^2 \leqslant 2\mu(H_{2j}) , \tag{3.55}$$

which shows that the bound on the right-hand side above is independent of k as long as $k \geqslant 2j$.

Recall that the operator K_0 is the Hamiltonian for a system of $2n$ harmonic oscillators, and that K_0^{-1} is a compact operator. Since, for $j = 0,1$, (3.55) may be written as

$$\|K_0^{-1}(K_0 G_k)\|_{L^2} \leqslant 2\mu(1) , \quad \|K_0 G_k\|_{L^2} \leqslant 2\mu(H_2) , \tag{3.56}$$

and since an L^2 ball of fixed radius is weakly compact, one may extract from the sequence $\{K_0 G_k\}$ a weakly convergent sequence. Finally, since compact operators map weakly convergent sequences to strongly convergent ones, the subsequence selected has the property that $K_0^{-1} K_0 G_k$ converges strongly in L^2 to some real-valued function G. The inequalities in (3.56) imply

$$\|G\|_{L^2} \leqslant 2\mu(1) . \tag{3.57}$$

Repeat the process for the subsequence $\{G_{k_l}\}$, only now use

$$\|K_0^{-1} K_0^2 G_k\| \leqslant 2\mu(H_2) , \quad \|K_0^2 G_k\| \leqslant 2\mu(H_4) . \tag{3.58}$$

(It may be necessary to discard the first term of the subsequence. This will not affect the argument at all.) One may again extract a subsequence for which $\{K_0^2 G_{k'}\}$ is weakly convergent, and so $\{G_{k'}\}$ and $\{K_0 G_{k'}\}$ are strongly convergent. A moment's reflection shows that again

$$G_{k'} \to G , \quad K_0 G_{k'} \to K_0 G ,$$

and

$$\|K_0 G\|_{L^2} \leqslant 2\mu(H_2) .$$

This process may be repeated indefinitely. Doing so shows that G is in the domain of K_0^j for all $j \geqslant 0$, and that

$$\|K_0^j G\|_{L^2} \leqslant 2\mu(H_j) . \tag{3.59}$$

It is well known that this implies that G must belong to $\mathscr{S}(\Gamma)$.[18]

I now want to show that $\rho = G \circ G$ solves the moment problem. Define the functional

$$\mu_G(A) = \int A(z) G \circ G(z)\, dz . \tag{3.60}$$

Since G is a real-valued Schwartz function, μ_G is an $\hbar$-positive S functional, and it belongs to S_t^* for all t. From the way I constructed G, I can pick a subsequence $\{G_{k'}\}$ that has the property that $\{G_{k'}\}$, $\{K_0 G_{k'}\}$,...,$\{K_0^j G_{k'}\}$ all converge in L^2 to G, $K_0 G$,...,$K_0^{j+1} G_{k'}$, respectively. One may also require that $2k' \geqslant j+1$, for doing so merely discards a finite number of terms in the sequence.

Let P be any polynomial of degree less than $2j+2$; obviously, P belongs to S_{2j+1}. In Corollary 3.11, put $\phi' = \mu_{k'}$ and $\phi = \mu_G$, note that $\mu_{k'}(P) = \mu(P)$, and use the bounds (3.55) and (3.59) in (3.54). The inequality (3.54) then becomes

$$|\mu(P) - \mu_G(P)| \leqslant 2\|T_{-4j-4}(P)\| \sqrt{\mu(H_{j+1})}\, \|K_0^{j+1}(G - G_{k'})\|_{L^2} . \tag{3.61}$$

As $k' \to \infty$ the right-hand side vanishes. The left-hand side is, however, independent of k' and so is 0 to begin with. Thus

$$\mu(P) = \mu_G(P) \tag{3.62}$$

for all polynomials of degree $2j+1$ or less. Finally, since the construction may be carried out for any j, one sees that (3.62) holds for all polynomials. If one sets $\rho = G \circ G$ and takes P to be any of the monomials in (1.3), then one see that (1.2) holds. [I remark that j above, unlike the j in (1.3), is just an integer; j in (1.3) is a multi-index.] This completes the proof.

The methods used above also yield sufficient conditions for the solution of a truncated moment problem in which one knows moments up to some fixed order.

Corollary 3.12: Suppose that one is given a set of numbers $m_{j,k}$, with $|j| + |k| \leqslant 2\nu + 2$, ν being a non-negative integer. A sufficient condition for the $m_{j,k}$'s to be of the form (1.2) for $|j| + |k| \leqslant 2\nu + 1$ is that the moment functional $\mu(P)$ be non-negative for every $\hbar$-positive polynomial P having degree $2\nu + 2$ or less.

Proof: Just apply Corollary 2.7, Theorem 3.2, and Proposition 3.10 to get a G for which (1.2) holds, at least in the sense of (3.51), for all polynomials of degree $2\nu + 1$ or less. One runs into difficulty with reproducing the highest order moments because the functional involved may have a term like ϕ_c in (3.52).

IV. CONCLUDING REMARKS

As I mentioned in Sec. I, O'Connell and I gave a set of necessary conditions for a sequence $\{m_{j,k}\}$ to be of the form (1.2).[2] If one examines that set, one easily sees that it is precisely the set of conditions obtained by requiring that the moment functional μ be non-negative on all $\hbar$-positive polynomials of the form $P \circ \overline{P}$. Whether this set is sufficient as well as necessary obviously hinges on whether *every* $\hbar$-positive polynomial may be written as a sum of polynomials of the form $P \circ \overline{P}$. In the classical, one-dimensional Hamburger moment problem, the analogous question would be whether every non-negative polynomial in one variable can be written as the sum of squares of polynomials. The answer is, of course, yes, and the set of conditions analogous to those of Ref. 2 are indeed sufficient.[19] For the classical, multidimensional problem, the answer is no,[20,21] and the corresponding set of conditions is *not* sufficient.[22] On the basis of the answer in the classical, multidimensional case, I conjecture that the conditions given in Ref. 2 are *not* sufficient. I do so with some hesitation, for there are many differences between the quantum mechanical moment problem treated here and the classical, multidimensional moment problem.

The set of restrictions imposed on the moments by requiring that the moment functional μ be non-negative for $\hbar$-positive polynomials has an interesting physical interpretation. If one sets

$$P = c_0 + \mathbf{c}_1 \cdot \mathbf{p} + \mathbf{c}_2 \cdot \mathbf{q} , \tag{4.1}$$

where c_0 is a complex number, and $\mathbf{c}_1$, $\mathbf{c}_2$ are in $\mathbb{C}^n$, then $\mu(P \circ \overline{P}) \geqslant 0$ gives rise to a quadratic form. Applying the stan-

dard conditions for this form to be non-negative results in the position-momentum uncertainty relations.[2] If one replaces P in (4.1) by an arbitrary polynomial, then $\mu(P\circ\overline{P})\geqslant 0$ is a non-negative quadratic form in the coefficients of P. The restrictions imposed on the moments in this case form a set of *generalized* uncertainty relations.[2] Should the conjecture I made above prove true, then there will be $\hbar$ polynomials that are *not* sums of polynomials of the form $P\circ\overline{P}$. The moment functional μ applied to such polynomials will give rise to additional restrictions on the moments, and so will augment that set of generalized uncertainty relations. In any case, one will arrive at a "complete set" of uncertainty relations for the moments. [By this I mean a set of restrictions satisfied if and only if the $m_{j,k}$'s are of the form (1.2). There are, of course, other uncertainty relations; see Breitenberger's paper[23] for a discussion.]

There are several interesting, unanswered questions concerning the quantum mechanical moment problem discussed here. The first is related to what polynomials are actually $\hbar$ positive. Voros[5] points out that every semibounded function in S_m gives rise to a semibounded operator on $L^2(\mathbb{R}^n)$. In particular, every non-negative polynomial in $\mathbf{q}$ and $\mathbf{p}$ can be made into an $\hbar$ positive one just by adding a positive constant to it. Is the converse also true? Put another way, does every $\hbar$-positive polynomial differ from a non-negative polynomial by a constant? If the answer is yes, then the difference between the quantum mechanical moment problem and the classical one is small indeed. The answer to this question might also shed light on the difference between states in quantum mechanics and in classical mechanics.

In proving sufficiency in Theorem 1.1, I merely showed that an appropriate Wigner function ρ existed. Is this function unique? If it is, the moments would serve as a kind of "minimal set" of expectation values required to determine ρ. Also, whether the solution is or is not unique, is there any method—say, some kind of variational procedure—for constructing ρ? Finally, is there a way of constructing solutions to the truncated moment problem mentioned in Corollary 3.12?

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Composite systems in quaternionic quantum mechanics

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The natural composition of systems in quaternionic quantum mechanics is examined via their lattices of propositions and it is shown that the criticisms that have been made of such a composition are unconvincing.

I. INTRODUCTION

Complex quantum mechanics is at the center of much of modern physics but in spite of this there remain unanswered fundamental questions about why it is preferred above alternative quantum theories. The need for an understanding of this preference is made more pertinent because of the important place phase invariance has taken in particle physics. Quaternionic quantum mechanics, the most prominent alternative, is considered here.

To quote Finkelstein *et al.* on quaternionic quantum mechanics, "The principal conceptual difficulty concerns the theory of composite systems where the ordinary tensor product fails due to noncommutativity."[1] Many authors working in the field since have agreed.[2–5] However, it is in response to this difficulty that Finkelstein *et al.* and the subsequent literature have diverged. While Finkelstein *et al.* considered that a sensible theory could be arrived at despite the requirement that the composite Hilbert space be quaternionic, the rest of the literature has asserted either that one must give up quaternionic quantum mechanics[2] or give up a quaternionic composite Hilbert space.[3,4]

What we hope to do here is to put forward a theory of composition in quaternionic quantum mechanics following Finkelstein *et al.* and then to show that the criticisms of such a program that are found in the literature are unconvincing.

The notions of quaternionic Hilbert space used here will be those of Horwitz and Biedenharn.[4]

II. QUATERNIONIC COMPOSITION

Following Aerts,[6] Zecca,[7] and Finkelstein *et al.*,[8] the composition of distinguishable quantum systems should be viewed as a lattice theoretic problem. Then we ask: given two quantum systems S_1 and S_2 and their corresponding lattices of propositions and sets of states $(\mathscr{L}_1, \mathscr{S}_1)$ and $(\mathscr{L}_2, \mathscr{S}_2)$, what quantum systems S, $(\mathscr{L}, \mathscr{S})$ may be considered as containing both S_1 and S_2? That is, what does it mean for one quantum system to contain two others? In line with the above three authors we are going to say it means that if you could ask a question of system 1 (e.g., the particle, that system 1 is, has a momentum p) as a system by itself then you can ask the same question of the composite system (e.g., that particle 1 has momentum p) and similarly for system 2. Mathematically this may be interpreted as the assertion that there exist mappings $h_i: \mathscr{L}_i \to \mathscr{L}$, for $i = 1, 2$, sending propositions of the subsystems to the corresponding, "the same," propositions in the composite system. This sameness of the elements in h_i $(\mathscr{L}_i)$ and the elements in $\mathscr{L}_i$ implies also that h_i preserves the structure of $\mathscr{L}_i$. We will call the existence of h_i and the preservation of the structure of $\mathscr{L}_i$ by h_i Axiom 1.

One might describe what has been done as finding a natural and directly interpretable axiom deductable from physically plausable assumptions, which is something that is always useful to do.[9]

It may be that this axiom is too strong to include all systems that we might like to call composite. Composition could possibly be better, or more generally, described via states or via maps from $\mathscr{L}$ to $\mathscr{L}_i$. However, what we are trying to do here is develop a definitive notion of composition. Axiom 1 will suffice.

Having asserted Axiom 1 we need to consider the relationship between h_1 and h_2 that is the relationship between the two components inside the composite. If we were to describe two completely independent subsystems then we would be able to give very strong requirements governing the relationship between h_1 and h_2 as do Aerts[6] and Aerts and Daubechies.[10] However, we have traditionally considered a wide range of systems as composite. Systems such as two balls on a string, the hydrogen atom, and three quarks bound by gluons are all different from the sum of the components acting independently.

If we follow wave mechanics where the position observables Q_1 and Q_2 are singled out as multiplication by x_1 and x_2, respectively, then there is a natural composite Hilbert space and a natural relationship between h_1 and h_2. For the case of one-dimensional particles the component Hilbert spaces are $L^2_Q(\mathbb{R})_1$ and $L^2_Q(\mathbb{R})_2$, the Lebesgue square integrable functions from R to Q, and the natural Hilbert space for the composite system, a system with two degrees of freedom, is $L^2_Q(\mathbb{R}^2)$. The lattice mappings h_1 and h_2 that Axiom 1 requires become mappings of closed subspaces of $L^2_Q(\mathbb{R})_i$ to closed subspaces of $L^2_Q(\mathbb{R}^2)$ for $i = 1,2$. Though it is not necessary it is both convenient and natural for these to take the form

$$\begin{aligned} h_1&: S_1 \subseteq L^2_Q(\mathbb{R})_1 \to \{\psi_1 \cdot \chi_2 : (x_1, x_2) \\ &\qquad \to \psi_1(x_1)\chi_2(x_2) \mid \psi_1 \in S_1,\ \chi_2 \in L^2_Q(\mathbb{R})_2\}, \\ h_2&: S_2 \subseteq L^2_Q(\mathbb{R})_2 \to \{\psi_2 \cdot \chi_1 : (x_1, x_2) \\ &\qquad \to \psi_2(x_2)\chi_1(x_1) \mid \psi_2 \in S_2,\ \chi_1 \in L^2_Q(\mathbb{R})_1\}. \end{aligned} \tag{1}$$

Observables, as lattice-valued measures, of the component systems may be associated with observables of the composite system via h_1 and h_2. If O an observable of system i maps E, a

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Borel subset of R, to $O(E)$ an element of $\mathscr{L}_i$, then the corresponding composite observable maps E to $h_i(O(E))$. Now as the spectral theorem applies unchanged to quaternionic Hilbert spaces we may express this association in terms of Hermitian operators. To do this we must first note that for all Φ an element of $L_Q^2(\mathbb{R}^2)$, $\Phi(x_1,x_2)$, may be written as a sum,

$$\sum_i \psi_i^1(x_1)\psi_i^2(x_2),$$

where $\psi_i^j \in L_Q^2(\mathbb{R})_j$ just as with the complex case. With this expression of elements of $L_Q^2(R)^2$ an operator A_1 of subsystem 1 can be associated with an operator A of the composite system via

$$(A\Phi)(x_1,x_2) = \sum_i (A_1\psi_i^1)(x_1)\psi_i^2(x_2). \tag{2}$$

This operator association sends projections onto S_1, a subspace of $L_Q^2(\mathbb{R})_1$ to projections onto $h_1(S_1)$ so that it corresponds to the association of lattice-valued measures given in Eq. (1). A similar association may be made between an operator A_2 of $L_Q^2(\mathbb{R})_2$ and a composite operator A,

$$(A\Phi)(x_1,x_2) = \sum_i (A_2\phi_i^2)(x_2)\phi_i^1(x_1), \tag{3}$$

which agrees with h_2, where

$$\sum_i \phi_i^2(x_2)\phi_i^1(x_1)$$

is an expansion of $\Phi(x_1,x_2)$ with elements of $L_Q^2(\mathbb{R})_2$ leading. In the composition given in Eq. (1) Q_1 commutes with all the observables of system 2 and similarly Q_2 with those of system 1. This is because both Q_1 and Q_2 send real functions to real functions: For $i = 1,2$ $(Q_i\Psi)(x_1,x_2) = x_i\psi(x_1,x_2)$. On the other hand, the momentum observables P_1 and P_2 do not in general commute with the observables of system 2 or system 1, respectively, in the way that Q_1 and Q_2 do. This is because P_1 is of the form $J_1(\partial/\partial x_1)$ with J_1 an anti-Hermitian unitary operator which commutes with $(\partial/\partial x_1)$ and J_1 defined from the time translation operator in system 1. And J_2 is similarly related to P_2 (Refs. 11 and 12). Here J_1 does not in general send real functions to real functions. This quaternionic nature of J_1 will neither allow it nor P_1 to commute with all the observables of system 2.

This whole discussion could have been carried out just as well with the component systems displayed in momentum space.[11] The Hilbert spaces would be the same function spaces but the association between Hermitian operators and physical observables would be different and h_1 and h_2 would not be given by Eq. (1). Here momentum observables P_1 and P_2 would have the form $(P_i\Psi)(p_1,p_2) = p_i\Psi(p_1,p_2)$ in the composite system. So P_1 would commute with all the observables of system 2 and similarly for P_2. The two compositions, one based on position and the other on momentum, are not equivalent. Finkelstein *et al.*[3,8] have indicated that each such representation of the component systems in terms of function spaces is a definition of what observables are real. So the choice of representation determines which observables of system 1 commute with which observables of system 2. So the choice determines the composite system. Which observables commute has direct physical consequences when observables are measured simultaneously. So in situations without superselection rules the choice of composition is determined by experiment.

We have shown in Ref. 11 that for quanternionic quantum mechanics (QQM) to be consistent with the remarkably successful description of the world provided by complex quantum mechanics (CQM) it must be that CQM is embedded in QQM. This has the effect that in the wave mechanics representation of system 1 $(J_1\phi_1)(x_1) = q_1\phi_1(x_1)$ for all $\phi_1 \in L_Q^2(\mathbb{R})_1$ for some fixed q_1 a pure imaginary quaternion of unit length. Similarly $J_2\phi_2(x_2) = q_2\phi_2(x_2)$ for all $\phi_2 \in L_Q^2(\mathbb{R})_2$ for some fixed q_2 a pure imaginary quaternion of unit length. With this restriction of the J's a complex quantum mechanics can be seen to be contained in each of the component systems.[11] Complex is defined for observables, states, and scalars via commutation with q_1 and q_2 in system 1 and system 2, respectively. Similarly we expect that "complex" may be defined for the composite system or may be induced from the components. The success of complex quantum mechanics, especially in its use of isolated systems, is strong evidence for the complex observables of system 1 to commute with the complex observables of system 2 at least when operating on complex composite states, which is sufficient to ensure that they do commute. It might be, however, that the commutator of complex observables from different systems is not zero but just small when acting on complex states of the composite system. We believe it would need to be vanishingly small and will not consider the possibility here.

The above requirement that the complex observables of different systems commute restricts the possible representations of the component systems. The wave mechanic representations of systems 1 and 2 must be such that $q_1 = q_2 = q$. Otherwise, in particular, $[P_1, P_2] \neq 0$. Similarly for the momentum representations where $Q_1 = q_1(\partial/\partial p_1)$ and $Q_2 = q_2(\partial/\partial p_2)$ it must be that $q_1 = q_2 = q$.

What is still left ill defined is the relationship between observables of the two systems when one of the observables is not complex. In particular, which if any complex observable of system 1 commutes with all observables of system 2. That this ambiguity remains is not so much the result of an ill defined composition procedure but the result of the hiddenness of quaternion quantum mechanics, since as we have said the choice of composition should be able to be determined by experiment. No measurement has ever been identified as being of a noncomplex observable nor of a noncomplex state. It is with such measurements that the precise nature of composition in quaternionic quantum mechanics must be determined. It also behooves quaternionic quantum mechanics to explain the lack of such experimental evidence, but we will avoid this issue here.

III. ARGUMENTS AGAINST QUATERNIONIC COMPOSITION

To our knowledge there have been two arguments given in the literature purporting to show that the composition of two subsystems described by quaternionic Hilbert spaces cannot in turn be described by a quaternionic Hilbert space.

One based upon lattice theoretic considerations is given by Aerts[2,6] and the other, based on Hilbert space ideas which mirror Aerts's work somewhat, is put forward by Rembielinski.[3]

Aerts describes a system S as composed of systems S_1 and S_2 if the three following conditions are satisfied.

(1) The structure of S_1 and S_2 is preserved when considered as parts of S.

(2) A measurement on one of the systems S_1 or S_2 does not disturb the other one.

(3) When we know the state of S_1 and of S_2 then we know also the state of S.

He then interprets these as the following lattice theoretic conditions.

(1′) There must exist maps h_1: $\mathscr{L}_1 \to \mathscr{L}$ and h_2: $\mathscr{L}_2 \to \mathscr{L}$, where h_1 and h_2 conserve the structure of $\mathscr{L}_1$ and $\mathscr{L}_2$.

(2′) If $a_1 \in \mathscr{L}_1$ and $a_2 \in \mathscr{L}_2$, then $h_1(a_1)$ is compatible with $h_2(a_2)$.

(3′) If a_1 is an atom of $\mathscr{L}_1$ and a_2 is an atom of $\mathscr{L}_2$ then $h_1(a_1) \wedge h_2(a_2)$ is an atom of $\mathscr{L}$.

Then in the language of generalized Hilbert spaces which represent $\mathscr{L}_1$, $\mathscr{L}_2$, and $\mathscr{L}$ Aerts proves some very general theorems asserting the existence of a bilinear (σ_1,σ_2) isometry from the component vector spaces to the composite vector space which preserves the composition provided by h_1 and h_2. These theorems have as their corollary that the Hilbert spaces representing each of the lattices may not all be over the quaternions.

That Aerts should come to such a conclusion is clear from the assumptions he makes. To show this we follow Finkelstein *et al.*[8] and note for $\psi_1 \in L^2_Q(\mathbb{R})_1$ and $\psi_2 \in L^2_Q(\mathbb{R})_2$ that

$$h_1(\{\psi_1\alpha\colon\ \alpha\in Q\}) \wedge h_2(\{\psi_2\beta\colon\ \beta\in Q\}) = \{\psi_1\cdot\chi_2\colon\ (x_1,x_2)\to\psi_1(x_1)\chi_2(x_2) \mid \chi_2\in L^2_Q(\mathbb{R})_2\} \wedge \{\psi_2\cdot\chi_1\colon\ (x_1,x_2)\to\psi_2(x_2)\chi_1(x_1) \mid \chi_1\in L^2_Q(\mathbb{R})_1\} \tag{4}$$

is nonempty if and only if there exist quaternions a and b such that $[\psi_1(x_1)a, \psi_2(x_2)b] = 0$ for all x_1 and x_2. As $\{\psi_1\alpha\colon \alpha\in Q\}$ and $\{\psi_2\beta\colon \beta\in Q\}$ are atoms of their respective lattices then the possibility of the above meet being null is in contradiction with 3′.

The assumptions 1,2,3 and their lattice theoretic interpretations 1′, 2′, 3′ are not only inconsistent with quaternionic composites but are similarly inconsistent with some simple complex compositions, in particular the complex quantum mechanics of two hard spheres and the quantum mechanics of two positively charged particles. Just as in quaternionic composition in the complex composition there are pairs of atomic propositions, namely, one from the quantum mechanics of one hard sphere (considered as a separate system) and the other from the quantum mechanics of the other hard sphere, for which the meet of the images of these propositions in the composite system is null. These are those pairs in which the two spheres are required to occupy some volume in common. The quaternionic and the hard sphere compositions are similar in that they both satisfy 1, 1′, and 3 for pure states but do not satisfy 2, 2′, and 3′. That they satisfy 1 and 1′ is clear. For 2 we note that most composite systems do not satisfy 2 in an unqualified way because there are always states of the composite system in which the component systems are correlated. The more specific and much less stringent requirement 2′ falls foul of both compositions because in each case there exist these propositions of each of the component systems whose meet in the composite system is null and such pairs can be found whose images in the composite system are not orthogonal. This is sufficient to prevent compatibility. For 3 and 3′ we see that when the meet of the images, in the composite system, of two atoms, one from each of the component systems, is not null then the meet is a uniquely determined atom of the composite system. So whenever we know what pure states S_1 and S_2 are in, and this is consistent with the two systems being composed together, then we know the state of S. In this way both compositions satisfy 3 but not 3′.

Rembielinski requires that composition be described by a vector product $f^1 \times f^2 \times \cdots \times f^r$ with f^k an element of the k th Hilbert space. This vector product is required to obey the distributivity condition $f^1 \times f^2 \times \cdots \times (g^k + h^k) \times \cdots \times f^r = f^1 \times f^2 \times \cdots \times g^k \times \cdots \times f^r + f^1 \times f^2 \times \cdots \times h^k \times \cdots \times f^r$ for every $k = 1$ to r. He notes that states are determined by rays and so requires $f^1 \times f^2 \times \cdots f^k\alpha \times \cdots \times f^r = (f^1 \times f^2 \times \cdots \times f^k \times \cdots \times f^r)\alpha^{\tau_k}$ for all k, where α is any element of the field of scalars of the component space and α^{C_k} is some element of the field of scalars of the product space. He is then able to show that the scalars of the component spaces commute, thus discounting Q. His argument depends crucially upon this relationship between rays of the component Hilbert spaces and those of the composite Hilbert space. In particular, the fact that the mapping τ_k is independent of f^1 to f^r. What we have considered in Sec. II is an alternative relationship, one not essentially based on Hilbert spaces but on lattices, so we have sidestepped his objection by never requiring the composition to be put in terms of individual vectors. It is interesting to note that the implementation of composition by a vector product is precisely what Aerts's theorems assure, so Rembielinski and Aerts have come to the same conclusions somewhat from the same direction.

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Component states of a composite quaternionic system

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The problem of finding component states given a composite state is examined for quaternionic quantum mechanics. It is shown that under very loose conditions the component state is forced to be complex.

I. INTRODUCTION

The problem of composing systems in quaternionic quantum mechanics (QQM) is one with many suggested solutions. Elsewhere[1] we have shown that the criticisms leveled against the natural solution that was first mooted by Finkelstein *et al.*[2] are insufficient to dismiss it and prompt a search for alternative and more elaborate solutions. It has become apparent[2–4] that the way to approach the problem is via the propositional lattices of the component systems and their embedding within that of the composite system. However, previous work[1,2] has only gone so far as to establish this embedding; what has not been discussed is the relationship between the states of the composite system and those of the component subsystems. This is what we propose to do here. In order to make the embedding and subsequent analysis more concrete we will discuss the composition of two one-dimensional quantum wave mechanical systems. That is, $L^2_Q(\mathbb{R})_1$ and $L^2_Q(\mathbb{R})_2$ will describe the component systems and $L^2_Q(\mathbb{R}^2)$ will describe the composite system. We will refer to these Hilbert spaces as H_1, H_2, and H, respectively, throughout this paper. These are of course sets of Lebegue square integrable functions from variously $\mathbb{R}$ and $\mathbb{R}^2$ to Q with the usual integral inner product. There is no preference for system 1 over system 2 as a component system of the composite system, so to avoid tiresome rewriting of results which focus upon one component system or upon the component systems differently, we note that in all that follows the subscripts or superscripts 1 and 2 may be interchanged.

Fortunately a number of useful structures carry over from complex quantum mechanics (CQM). We know that the states of these systems correspond to density operators acting on the corresponding Hilbert spaces just as in CQM because Gleason's theorem applies unchanged to quaternionic Hilbert spaces.[5,6] Also the spectral theorem remains unchanged[6] so observables are self-adjoint operators and may be expanded in terms of projection operators. Similarly the relationship between pure and mixed states is preserved, the latter as convex combinations of the former. Finally as an upshot of all this the probability that a proposition P_M, a projection onto the subspace M, is true when the system is in the state D, a density operator, is $\mathrm{tr}(DP_M)$.

The superscripts and subscripts 1,2, or nothing will denote things pertaining to system 1, system 2, or the composite system, respectively, in the following way: functions will be superscripted and inner products will be subscripted.

II. TWO QUESTIONS

There are two questions one can ask of the relationship between composite and component states. First, if the composite system is in a specified state D, what states if any can the component systems be in? Second, if we specify the states of the component systems what states if any can the composite system be in? To answer these questions we must form a criterion with which to say it is consistent for a component system (call it 1) to be in a state D_1 while the composite system is in a state D. Such a criterion is as follows: for any proposition of subsystem 1 the probability of that proposition being true, when subsystem 1 is in state D_1, is equal to the probability that the "same" proposition, as a proposition of the composite system, is true when the composite system is in state D.

Now the association between a proposition of the component system and the same proposition of the composite system is given by the embedding of the propositional lattice of the component system into that of the composite system as we discussed earlier. In Ref. 1 we argue that this embedding depends upon the choice of representation of the lattice of propositions of the two component systems within their Hilbert spaces. That is, it depends upon which subspaces represent which propositions or equivalently which Hermitian operators represent which physical observables. However, whichever representations are chosen the Hilbert spaces are still the same function spaces and, considered on these function spaces independent of interpretation, the embedding is fixed. So by putting off the discussion of observables for a moment we are free to discuss the embedding and its consequences for the relationship between the states, but without physical interpretation of the states. The embedding is as follows: if P_{M_1} is a proposition of the composite system 1, M_1 a subspace of H_1, then P_M is the same proposition in the composite system when $M = \{\phi^1 \cdot \psi^2 : \phi^1 \in M_1, \psi^2 \in H_2\}$, where $\phi^1 \cdot \psi^2 : (x_1, x_2) \to \phi^1(x_1)\psi^2(x_2)$.

So for D_1 and D states of the component and composite systems, respectively, to be consistent with each other we require that

$$\mathrm{tr}(D_1 P_{M_1}) = \mathrm{tr}(DP_M)$$

for all M_1 a subspace of H_1 [call this requirement (A)].

For further work we need the explicit form of P_M for a given M_1. Let $\{\chi^1_k\}$ be an orthonormal basis of M_1 and let $\{\xi^2_j\}$ be a real orthonormal basis of H_2 then $\{\chi^1_k \cdot \xi^2_j\}$ is an orthonormal basis of M. So for $\Psi \in H$,

$$P_M \Psi = \sum_{jk} \chi^1_k \cdot \xi^2_j (\chi^1_k \cdot \xi^2_j, \Psi) .$$

We always can write Ψ as

$$\sum_i \phi^1_i \cdot \psi^2_i a_i ,$$

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where $\phi_i^1 \in H_1$, $\psi_i^2 \in H_2$, and $a_i \in Q$ for all i. Thus using the properties of the inner products,

$$P_M \Psi = \sum_i (P_{M_1} \phi_i^1) \cdot \psi_i^2 a_i \,. \tag{1}$$

III. FIRST QUESTION

To answer the first question mentioned above we need to start with a state of the composite system D. Then given D, requirement (A) amounts to specifying a probability measure on the propositions of H_1, namely, $P_{M_1} \to \mathrm{tr}(DP_M)$. So Gleason's theorem asserts that some D_1 exists such that $\mathrm{tr}(D_1 P_{M_1}) = \mathrm{tr}(DP_M)$ for all M_1 and its corresponding M. We may also show that such a D_1 is unique. Suppose D_1' also satisfies $\mathrm{tr}(D_1' P_{M_1}) = \mathrm{tr}(DP_M)$ for all M_1, then $\mathrm{tr}(D_1' M_1) = \mathrm{tr}(D_1 M_1)$ for all M_1. Now for M_1 one-dimensional, $M_1 = \langle v \rangle$, this becomes $(v, D_1 v) = (v, D_1' v)$ for all $v \in H_1$. So writing $A = D_1 - D_1'$ we note that A is Hermitian and $(v, Av) = 0$ for all v. Take $u \in H_1$ then

$$\begin{aligned} 0 &= (Au + u, A(Au + u)) \\ &= (Au, A^2 u) + (u, A^2 u) + (Au, Au) + (u, Au) \\ &= 2\|Au\|^2 \,. \end{aligned} \tag{2}$$

Thus, $Au = 0$ for any $u \in H_1$ implying $D_1' = D_1$. Note that $\mathrm{tr}(D_1 P_{M_1})$ for one-dimensional propositions was sufficient to determine D_1 uniquely.

Having now shown the existence and uniqueness of D_1 one may reduce the problem. Any D a state of the composite system can be written as $\Sigma_i \alpha_i D^i$, where the D^i are pure states of the composite system. For each of these D^i we have D_1^i the unique solution to $\mathrm{tr}(D_1^i P_{M_1}) = \mathrm{tr}(D^i P_M)$ for all M_1. It is easily shown that $D_1 = \Sigma_i \alpha_i D_1^i$ satisfies condition (A) uniquely. Thus the problem is reduced to finding the component states corresponding to a pure composite state. We can solve this reduced problem. For D pure then $D = P_{\langle \Phi \rangle}$ the projection onto the one-dimensional subspace of H. Here $\langle \Phi \rangle = \{\Phi\alpha : \alpha \in Q\}$, where Φ is a unit element of H. Now Φ can always be written as $\Sigma_i \phi_i^1 \cdot \psi_i^2 \lambda_i$, where $\{\psi_i^2\}$ is a real orthonormal set in H_2, $\phi_i^1 \in H_1$, and $\lambda_i \in Q$ for all i. As we have shown above to uniquely determine D_1 it is sufficient to consider one-dimensional subspaces $M_1 = \{\chi^1 \alpha : \alpha \in Q\} = \langle \chi^1 \rangle$ for $\chi^1 \in H_1$ of unit length. Then for the corresponding M using Eq. (1) and the fact that the ψ_j^2 are real,

$$\begin{aligned} \mathrm{tr}(DP_M) &= \sum_{ij} \lambda_i^* (\psi_i^2, (\phi_i^1, \chi^1)_1 (\chi^1, \phi_j^1)_1 \psi_j^2)_2 \lambda_j \,, \\ &= \sum_i \lambda_i^* \lambda_i |(\phi_i^1, \chi^1)_1|^2 \,. \end{aligned} \tag{3}$$

Then it is easily shown that

$$D_1 = \sum_i \lambda_i^* \lambda_i P_{\langle \phi_i^1 \rangle}$$

satisfies condition (A) uniquely.

IV. SECOND QUESTION

Given states of the component systems D_1 and D_2 then D, a consistent state of the composite system, is neither guaranteed to be unique nor guaranteed to exist. The lack of uniqueness comes about just as it does in complex theories.[6,7] The possible nonexistence of a consistent D is new. This can be traced directly to the correspondence between propositions in the component systems and those in the composite system. The pertinent property is that via this correspondence the meet of some propositions of system 1 with some propositions of system 2 is null.

We can give an account of what happens in the restricted case where D_1 and D_2 are pure. If D exists and is mixed then from what has been said above D_1 and D_2 would have to be mixed. So we know that when it exists D is pure. Suppose D exists and let $D_1 = P_{\langle \phi^1 \rangle}$, $D_2 = P_{\langle \psi^2 \rangle}$, and $D = P_{\langle \Phi \rangle}$, where ϕ^1, ψ^1, and Φ are elements of H_1, H_2, and H, respectively, and are all of unit norm. Here Φ can always be written as $\Sigma_i \phi_i^1 \cdot \psi_i^2 \lambda_i$, where ϕ_i^1 is a unit element of H_1 and $\lambda_i \in Q$ for all i and where $\{\psi_i^2\}$ is a real orthonormal set in H_2. Thus from Sec. III

$$P_{\langle \phi^1 \rangle} = D_1 = \sum_i \lambda_i^* \lambda_i P_{\langle \phi_i^1 \rangle} \,. \tag{4}$$

Further if $v \in \langle \{\phi_i^1\} \rangle$ and $(v, \phi^1) = 0$ then

$$(v, P_{\langle \phi^1 \rangle} v) = 0 \neq \left(v, \sum_i \lambda_i^* \lambda_i P_{\langle \phi_i^1 \rangle} v \right).$$

This is a contradiction, so $\langle \{\phi_i^1\} \rangle = \langle \phi^1 \rangle$ and therefore $\phi_i^1 = \phi^1 \mu_i$ for some $\mu_i \in Q$ and for all i. Therefore

$$\Phi = \sum_i \phi^1 \mu_i \cdot \psi_i^2 \lambda_i = \phi^1 \cdot \sum_i \psi_i^2 \mu_i \lambda_i \,. \tag{5}$$

Similarly $\Phi = \psi^2 \cdot \chi^1$ for some $\chi^1 \in H_1$.

Finkelstein *et al.* have shown that Φ can be expressed in these two ways only if for some $\alpha, \beta \in Q$ $[\phi^1(x_1)\alpha, \psi^2(x_2)\beta] = 0$ for all x_1 and x_2 (Ref. 2). And in that case $\Phi = \phi^1 \gamma \cdot \psi^2 \delta$ for some $\gamma, \delta \in Q$. So these conditions are necessary conditions for D to exist. When these conditions are satisfied $D = P_{\langle \phi^1 \gamma \cdot \psi^2 \rangle}$ for some $\gamma \in Q$, so from the discussion in Sec. III they are sufficient conditions for D to exist. The above necessary and sufficient conditions are precisely the conditions for the propositions corresponding to $P_{\langle \phi^1 \rangle}$ and $P_{\langle \psi^2 \rangle}$ in the composite system to have a non-null meet.[2] So D exists when the atomic propositions that correspond to the pure states of the components have a non-null meet.

V. HIDDEN QQM

The thrust of this work is to show that QQM is hidden. To do this we must take a specific orientation of the physical observables within the component Hilbert spaces. We require in particular that the position observables Q_i have the form

$$(Q_i \phi^i)(x_i) = x_i \phi^i(x_i), \quad i = 1,2,$$

and that the momentum observables P_i have the form

$$(P_i \phi^i)(x_i) = e_1 \frac{\partial}{\partial x_i} \phi^i(x_i), \quad i = 1,2 \,.$$

That these observables can be written like this is shown in Ref. 8. The complex numbers are then defined as $\langle \{1, e_1\} \rangle = \{\alpha 1 + \beta e_1 : \alpha, \beta \in \mathbb{R}\}$ and the complex vectors in the function spaces H_1 and H_2 are those functions that map onto the complex subset of Q. We further show in Ref. 8 that

we can associate those states of QQM that leave the subset containing the complex vectors of the Hilbert space invariant with states of a CQM.

A. An illustration

We will now illustrate how it comes about that QQM might be hidden. Consider $D = P_{\langle\Phi\rangle}$ a state of the composite system $\Phi \in H$ with $\Phi(x_1,x_2) = \phi^1(x_1)\psi^2(x_2)$, ψ^2 a unit element of H_2 and $\phi^1 = (1/\sqrt{2})(\phi_1^1 + e_1\phi_2^1)$ for ϕ_1^1 and ϕ_2^1 real and unit elements of H_1, $(\phi_1^1,\phi_2^1)_1 = 0$. So we may write Φ as $\psi^2 \cdot \phi_1^1(1/\sqrt{2}) + e_1\psi^2 \cdot \phi_2^1(1/\sqrt{2})$ and then from our previous analysis

$$D_2 = \tfrac{1}{2}P_{\langle\psi^2\rangle} + \tfrac{1}{2}P_{\langle e_1\psi^2\rangle} . \tag{6}$$

We examine the action of D_2 on a complex element of H_2,

$$\begin{aligned} D_2\chi^2 &= \tfrac{1}{2}\psi^2(\psi^2,\chi^2)_2 + \tfrac{1}{2}e_1\psi^2(e_1\psi^2,\chi^2)_2 , \\ &= \tfrac{1}{2}\psi^2(\psi^2,\chi^2)_2 + \tfrac{1}{2}e_1\psi^2(\psi^2,\chi^2)_2 e_1^* \\ &\quad \text{as} \quad \chi^2(x_2) = \langle\{1,e_1\}\rangle \quad \text{for all } x_2 , \\ &= \psi_1^2 + e_1\psi_1^2 e_1^*, \quad \text{where } \psi_1^2 = \tfrac{1}{2}\psi^2(\psi^2,\chi^2)_2 . \end{aligned} \tag{7}$$

Therefore $D_2\chi^2$ is a complex element of H_2. So D_2 leaves the subset $L^{\,2}_{\langle\{1,e_1\}\rangle}(\mathbb{R})_2$ of H_2 invariant. Thus D_2 may be written as $\Sigma_i \alpha_i P_{\langle\xi_i^2(x_2)\rangle}$, where the $\xi_i^2(x_2)$ are complex functions in H_2 (Ref. 8). Thus for composite states of the form of D the component states of particle 2 are always complex, independent of the form of $\psi^2(x_2)$. So for such states their quaternionic nature is somewhat hidden.

Pursuing the illustration further we note that the power of the result we have obtained depends very much upon how many and which composite states are of the appropriate form. Apart from the fact that it is not normalizable the momentum state[8] $\exp(e_1 p x_1)$ would have the appropriate form for $\phi^1(x_1)$. However, in the case where we consider states normalized in a box of finite volume, $\phi^1(x_1) = (1/N)\exp(px_1)$ is a normalized vector for some $N \in R$. Hence

$$\begin{aligned} \Phi(x_1,x_2) &= \phi^1(x_1)\psi^2(x_2) \\ &= (1/\sqrt{2}N)\psi^2(x_2)\sqrt{2}\cos(px_1) \\ &\quad + (1/\sqrt{2}N)e_1\psi^2(x_2)\sqrt{2}\sin(px_1) \end{aligned} \tag{8}$$

is of the appropriate form for any $\psi^2 = L^{\,2}_Q(\mathrm{Box})_2$. It is clear that as well as D_2 being complex D_1 is the momentum state $P_{\langle(1/N)\exp(e_1 px)\rangle}$. This shows, for such a normalization, that a large class of composite states are of the appropriate form, including those in which D_1 is a momentum state. It is instructive for generalization to note that

$$\phi^1(x_1) = \tfrac{1}{2}(\exp(e_1 px_1) + \exp(-e_1 px_1)) = \cos(px_1)$$

does not leave $\Phi(x_1,x_2)$ in the appropriate form, as

$$\Phi(x_1,x_2) = \phi^1(x_1)\psi^2(x_2) = \psi^2(x_2)\cos(px_1)$$

and so $D_2 = P_{\langle\psi^2(x_2)\rangle}$.

B. A generalization

With the above in mind we examine a composite state $D = D_{\langle\Phi\rangle}$, where $\Phi(x_1,x_2) = \phi^1(x_1)\psi^2(x_2)$, ϕ^1 a unit element of H_1 and ψ^2 a unit element of H_2. We also require

$$\phi^1(x_1) = \left(\frac{1}{2\pi}\right)^{1/2}\int_{-\infty}^{\infty}\exp(e_1 p_1 x_1)\tilde{\phi}^1(p_1)dp_1$$

with $\tilde{\phi}(p_1) \neq 0$, implying $\tilde{\phi}^1(-p_1) = 0$ for which we will say $\tilde{\phi}^1$ satisfies condition (B). We will say D satisfies (B'). Then setting

$$A^1 = \left(\frac{1}{2\pi}\right)^{1/2}\int_{-\infty}^{\infty}\cos(p_1 x_1)\tilde{\phi}^1(p_1)dp_1$$

and

$$B^1 = \left(\frac{1}{2\pi}\right)^{1/2}\int_{-\infty}^{\infty}\sin(p_1 x_1)\tilde{\phi}^1(p_1)dp_1 ,$$

we may write

$$\Phi(x_1,x_2) = A^1(x_1)\psi^2(x_2) + e_1 B^1(x_1)\psi^2(x_2) . \tag{9}$$

Note that A^1 and B^1 are elements of H_1, A^1 is even, and B^1 is odd. If we can write

$$B^1(x_1) = \sum_i \chi_{Bi}^1(x_1)b_i$$

with $\{\chi_{Bi}^1\}$ an orthonormal set of real odd functions in H_1 and $b_i \in Q$ for all i and if we can also write

$$A^1(x_1) = \sum_i \chi_{Ai}^1(x_1)a_i$$

with $\{\chi_{Ai}^1\}$ an orthonormal set of real even functions in H_1 with $a_i = b_i$ for all i then

$$\begin{aligned} \Phi(x_1,x_2) &= \sum_i \frac{b_i}{|b_i|}\psi^2(x_2)\chi_{Ai}^1(x_1)|b_i| \\ &\quad + \sum_i e_1\frac{b_i}{|b_i|}\chi_{Bi}^1(x_1)|b_i| . \end{aligned} \tag{10}$$

Thus as $(\chi_{Ai}^1,\chi_{Bj}^1)_1 = 0$ for all i and j we have, from our previous discussion,

$$D_2 = \sum_i |b_i|^2(P_{\langle(b_i|b_i|)\psi^2\rangle} + P_{\langle e_1(b_i|b_i|)\psi^2\rangle}) , \tag{11}$$

which as before means that D_2 is complex.

We now need to show that we can find such sets $\{\chi_{Bi}^1\}$ and $\{\chi_{Ai}^1\}$. Take any orthonormal set of real odd functions $\{\chi_{Bi}^1\}$ that span the subspace of odd functions of H_1; then as B^1 is odd

$$B^1(x_1) = \sum_i \chi_{Bi}^1(x_1)b_i \quad \text{with} \quad b_i = (\chi_{Bi}^1,B^1)_1 .$$

We wish to find an orthonormal set of real even functions $\{\chi_{Ai}^1\}$ such that

$$A^1(x_1) = \sum_i \chi_{Ai}^1(x_1)a_i$$

with $a_i = (\chi_{Ai}^1,A^1)$ and $a_i = b_i$.

We may write

$$\chi_{Bi}^1(x_1) = \left(\frac{2}{\pi}\right)^{1/2}\int_{-\infty}^{\infty}\tilde{\chi}_{Bi}^1(p)\sin(px_1)dp$$

with $\tilde{\chi}_{Bi}^1(p) = 0$ for $p < 0$ as χ_{Bi}^1 is odd. Evaluating b_i we find that

$$b_1 = \int_0^\infty \tilde{\chi}^1_{Bi}(p)\tilde{\phi}^1(p)dp - \int_0^\infty \tilde{\chi}^1_{Bi}(p)\tilde{\phi}^1(-p)dp\,, \qquad (12)$$

by expanding the integrals. Now let $m_1 = \{p|\tilde{\phi}^1(p)\neq 0, p\geqslant 0\}$ and $m_2 = \{p|\tilde{\phi}^1(-p)\neq 0, p\geqslant 0\}$ then by condition (B) $m_1 \cap m_2 = \phi$. Further, take any $M_1 \supseteq m_2$ and $M_2 \supseteq m_2$ such that $M_1 \cup M_2 = R^+ \cup \{0\}$ and $M_1 \cap M_2 = \phi$, then

$$b_i = \int_{M_1} \tilde{\chi}^1_{Bi}(p)\tilde{\phi}^1(p)dp - \int_{M_2} \tilde{\chi}^1_{Bi}(p)\tilde{\phi}^1(-p)dp\,.$$

Similarly we may write

$$\chi^1_{Ai}(x_1) = \left(\frac{2}{\pi}\right)^{1/2} \int_{-\infty}^{\infty} \tilde{\chi}^1_{Ai}(p)\cos(px_1)dp$$

with $\tilde{\chi}^1_{Ai}(p) = 0$ for $p<0$ as χ^1_{Ai} is even. And similarly we may evaluate a_i,

$$a_i = \int_{M_1} \tilde{\chi}^1_{Ai}(p)\tilde{\phi}^1(p)dp + \int_{M_2} \tilde{\chi}^1_{Ai}(p)\tilde{\phi}^1(-p)dp\,. \qquad (13)$$

So to ensure $a_i = b_i$ it is sufficient to demand that $\chi^1_{Ai}(x_1)$ satisfy $\tilde{\chi}^1_{Ai}(p) = \tilde{\chi}^1_{Bi}(p)$ for $p\in M_1$, $\tilde{\chi}^1_{Ai}(p) = -\tilde{\chi}^1_{Bi}(p)$ for $p\in M_2$, and $\tilde{\chi}^1_{Ai}(p) = \tilde{\chi}^1_{Bi}(p) = 0$ for $p<0$.

We have left to show that $\{\chi^1_{Ai}\}$ is an orthonormal set of real even functions in H_1. That $\chi^1_{Ai}(x_1)$ is even is obvious since it has a cosine expansion. That $\chi^1_{Ai}(x_1)$ is real is ensured by $\tilde{\chi}^1_{Ai}(p)$ being real which in turn comes from $\chi^1_{Bi}(x_1)$ being real. Using the above relationship between $\tilde{\chi}^1_{Ai}(p)$ and $\tilde{\chi}^1_{Bi}(p)$ it is easy to show that

$$(\chi^1_{Ai},\chi^1_{Aj}) = (\chi^1_{Bi},\chi^1_{Bj})\,. \qquad (14)$$

Thus $\chi^1_{Ai}(x_1)$ is square integrable for all i and $\{\chi^1_{Ai}(x_1)\}$ is an orthonormal set in H_1. So D_2 is complex whenever D satisfies (B′).

C. Superpositions

We will extend this result to superpositions, that is to states $D_{\langle\Phi\rangle}$ with

$$\Phi(x_1,x_2) = \sum_i \phi^1_i(x_1)\psi^2_i(x_2)\,,$$

where

$$\phi^1_i(x_1) = \left(\frac{1}{2\pi}\right)^{1/2} \int_{-\infty}^{\infty} \exp(e_1 p_1 x_1)\tilde{\phi}^1_i(p)dp$$

and where $\tilde{\phi}^1_i(p)\neq 0$ for some i implies $\tilde{\phi}^1_j(-p) = 0$ for all j. We will say $\{\tilde{\phi}^1_i\}$ satisfies condition (C), and that D satisfies condition (C′).

We may write $\Phi(x_1,x_2)$,

$$\begin{aligned}\Phi(x_1,x_2) &= \sum_i \left(\frac{1}{2\pi}\right)^{1/2} \int_{-\infty}^{\infty} \exp(e_1 p_1 x_1)\tilde{\phi}^1_i(p)dp\,\psi_i(x_2)\,,\\ &= \left(\frac{1}{2\pi}\right)^{1/2} \sum_i \left(\int_{-\infty}^{\infty} \tilde{\phi}^1_i(p)\cos(px_1)dp\,\psi_i(x_2)\right.\\ &\quad \left. + e_1 \int_{-\infty}^{\infty} \tilde{\phi}^1_i(p)\sin(px_1)dp\,\psi_i(x_2)\right)\\ &= \sum_i A^1_i(x_1)\psi_i(x_2) + \sum_i e_1 B^1_i(x_1)\psi_i(x_2)\,. \qquad (15)\end{aligned}$$

Then if we can write

$$B^1_i(x) = \sum_j \chi^1_{Bj}(x_1)b_{ij}$$

with $\{\chi^1_{Bj}\}$ an orthonormal set of real odd functions in H_1 and if we can also write

$$A^1_i(x_1) = \sum_i \chi^1_{Aj}(x_1)a_{ij}$$

with $\{\chi^1_{Aj}\}$ an orthonormal set of real even functions in H_1 and $a_{ij} = b_{ij}$ for all i and j we have

$$\begin{aligned}\Phi(x_1,x_2) = \sum_j \Bigg(&\frac{(\Sigma_i b_{ij}\psi^2_i(x_2))}{N_j}\chi^1_{Aj}(x_1)N_j\\ &+ e_1 \frac{(\Sigma_i b_{ij}\psi^2_i(x_2))}{N_j}\chi^1_{Bj}(x_2)N_j\Bigg)\,, \qquad (16)\end{aligned}$$

with

$$N_j = \left|\left|\sum_i b_{ij}\psi_i(x_2)\right|\right|\,.$$

So as $(\chi^1_{Aj}(x_1),\chi^1_{Bi}(x_1)) = 0$ for all i and j we have that

$$D_2 = \sum_j (P_{\langle\Sigma_i(a_{ij}\psi^2_i/N_j)\rangle} + P_{\langle e_1\Sigma_i(b_{ij}\psi^2_i/N_j)\rangle})\,, \qquad (17)$$

which, as before, is complex.

To show that we can find the required orthonormal sets we note that $\{\tilde{\phi}^1_i\}$ satisfying condition (C) implies that the non-negative real line may be split into two disjointed sets M_1 and M_2 with

$$M_1 \supseteq \{p:\ \tilde{\phi}^1_i(p)\neq 0,\ p\geqslant 0\} \text{ for all } i$$

and

$$M_2 \supseteq \{p:\ \tilde{\phi}^1_i(-p)\neq 0,\ p\geqslant 0\} \text{ for all } i\,.$$

So given $\{\chi^1_{Bj}\}$ an orthonormal set of real odd functions we may define $\{\chi^1_{Aj}\}$ as before via M_1 and M_2 which we note are independent of i. So for each i the required conditions to show $a_{ij} = b_{ij}$ for all j are satisfied by this choice of $\{\chi^1_{Bj}\}$ and $\{\chi^1_{Aj}\}$.

D. Momentum conditions

We will now show that a pure composite state satisfying condition (C′) is equivalent to the probability density Pd of the momentum of particle 1 satisfying condition (B).

First take $D = P_{\langle\Phi\rangle}$ with

$$\Phi(x_1,x_2) = \sum_i \phi^1_i(x_1)\psi^2_i(x_2)$$

and

$$\psi^2_i(x_2) = \sum_j \xi^2_j(x_2)\lambda_{ji}\,,$$

where $\{\xi^2_j\}$ is an orthonormal set of real functions and a basis for H_2 and $\lambda_{ji}\in Q$ for all i and j. Then

$$\Phi(x_1,x_2) = \sum_{ji} \phi^1_i(x_1)\lambda_{ji}\xi^2_j(x_2)\,.$$

Thus the component state

$$D_1 = \sum_j \alpha_j P_{\langle\Sigma_i\phi^1_i\lambda_{ij}\rangle}\,,$$

where

$$\alpha_j = \left|\left| \sum_i \phi_i^1(x_1)\lambda_{ji} \right|\right| .$$

The particle 1 momentum probability density function $\mathrm{Pd}(p)$ is then

$$\sum_j \alpha_j^2 \left(\sum_i \tilde{\phi}_i^1(p)\lambda_{ji}\right)^* \left(\sum_i \tilde{\phi}_i^1(p)\lambda_{ji}\right).$$

Suppose D satisfies (C'). So condition (C) holds for $\{\tilde{\phi}_i^1\}$. Take $p \in \mathbf{R}$ if $\mathrm{Pd}(p) \neq 0$, then $\tilde{\phi}_i^1(p) \neq 0$ for some i; thus we have that $\tilde{\phi}_k^1(-p) = 0$ for all k. It follows that $\mathrm{Pd}(-p) = 0$. Therefore Pd satisfies condition (B).

On the other hand suppose Pd satisfies (B), i.e., $\mathrm{Pd}(p) \neq 0$ implies $\mathrm{Pd}(-p) = 0$. Then

$$\sum_i \tilde{\phi}_i^1(p)\lambda_{ji} \neq 0$$

for some j forces

$$\sum_i \tilde{\phi}_i^1(-p)\lambda_{ji} = 0$$

for all j. So letting

$$f_j^1(x_1) = \sum_i \phi^1(x_1)\lambda_{ji}$$

we have that

$$\Phi(x_1,x_2) = \sum_j f_j^1(x_1)\xi_j^2(x_2)$$

with $\{\tilde{f}_j^1\}$ satisfying condition (C) as

$$\tilde{f}_j^1(p) = \sum_i \tilde{\phi}_i^1(p)\lambda_{ji} .$$

So D satisfies (C').

Finally consider a nonpure state $D = \Sigma_i \alpha_i D_i$, D_i pure, with the particle 1 momentum probability density function $\mathrm{Pd}(p)$ satisfying condition (B). As

$$\mathrm{Pd}(p) = \sum_i \alpha_i^2 \mathrm{Pd}^i(p) ,$$

Pd^i the particle 1 momentum probability density function for state D^i also satisfies condition (B) for all i. It follows that D^i satisfies (C') and therefore that D_2^i is complex and, as convex combinations of complex states are complex, that D_2 is complex.

We have then that for any composite state D if the probability density function for the momentum of particle 1 satisfies condition (B) then the component state of particle 2, D_2, is complex. Extending this result to three dimensions and to many particles is just a matter of introducing new parameters and may be derived as a corollary to the two-particle, one-dimensional case. The statement of the theorem then becomes, that for any many particle three-dimensional state D, if the probability density function for the component of the momentum in any direction of any particle satisfies condition (B) then the component system of the rest of the particles together is complex. That condition (B) is satisfied by a momentum probability density is a common situation. For instance, (B) is satisfied if any component of the momentum of a particle is entirely positive. This occurs whenever the momenta of all but one of the products of a decay are measured sufficiently accurately which, for the two-body decay, amounts to observing one of the particles to be within any hemisphere centered on the center of mass.

VI. CONCLUSION

We have found that the description of the component states for a given composite state follows along much the same lines as in complex quantum mechanics. Using this formalism we have shown that the component states are complex under weak conditions, much weaker than requiring one particle to be a momentum state. This means that if one can only measure component systems then it is plausible for the component system to be always in a complex state while the total system is in a quaternionic state, thus shielding quaternionic states from investigation.

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Absolutely continuous spectra of quasiperiodic Schrödinger operators

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Several aspects of the general and constructive spectral theory of quasiperiodic Schrödinger operators in one dimension are discussed. An explicit formula for the absolutely continuous (a.c.) spectral densities that yields an immediate proof of the fact that the Kolmogorov–Arnold–Moser (KAM) spectrum constructed by Dinaburg, Sinai, and Rüssmann [Funkt. Anal. Prilozen. **9**, 8 (1975); Ann. Acad. Sci. **357**, 90 (1980)] is a subset of the a.c. spectrum is provided. Some quasiperiodicity properties of the Deift–Simon a.c. eigenfunctions are proved, namely, that the normalized phase of such eigenfunctions is a quasiperiodic distribution. In the constructive part the Dinaburg–Sinai–Rüssmann theory is extended to quasiperiodic perturbations of periodic Schrödinger operators using a KAM Hamiltonian formalism based on a new treatment of perturbations of harmonic oscillators. Particular attention is devoted to the dependence upon the eigenvalue parameter and a complete control of KAM objects is achieved using the notion of Whitney smoothness.

I. INTRODUCTION

Let L_θ be a quasiperiodic Schrödinger operator in one dimension,[1–6]

$$L_\theta \equiv L(v_\theta) \equiv -\frac{d^2}{dx^2} + v_\theta(x),$$

$$v_\theta(x) \equiv V(T_x\theta), \quad T_x\theta \equiv \theta + \omega x,$$

where $x \in \mathbb{R}$, $\theta \in \mathbb{T}^d \equiv \mathbb{R}^d/2\pi\mathbb{Z}^d$, $\omega \in \mathbb{R}^d$ is a rationally independent vector and V is a real function defined on $\mathbb{T}^d$. In this paper we discuss, from two points of view, the absolutely continuous (a.c.) spectrum of L_θ. First, continuing the analysis in Refs. 2, 3, and 7, we study some general problems such as characterization almost everywhere (with respect to Lebesgue measure on $\mathbb{R}$ and/or Haar measure on $\mathbb{T}^d$) of the a.c. eigenfunctions and of spectral densities. Then we turn to the explicit construction of many (in the sense of Lebesgue measure) quasiperiodic a.c. eigenfunctions for a special class of potentials v. This second part should be regarded as a refinement of the theory in Refs. 8 and 9.

Our results in the general part are described by the following three theorems. Before describing them let us recall a few definitions. The spectral class measure $d\mu^\theta$ is given by one of the following mutually equivalent measures:

$$d\mu^\theta = \sum_1^\infty a_n \, d\mu^\theta_{\phi_n}, \quad a_n > 0, \quad \phi_n \in C_0^\infty,$$

where $\Sigma a_n < \infty$, $\{\phi_n\}$ is an L^2-dense set of C^∞ functions with compact support and $d\mu^\theta_{\phi_n}$ denotes the standard spectral measure of L_θ based upon ϕ_n. Now let $d\mu^\theta_{\text{a.c.}}$ be the a.c. part of $d\mu^\theta$ in the Jordan–Lebesgue decomposition. The essential support S of $d\mu^\theta_{\text{a.c.}}$ is uniquely determined (modulo sets of zero Lebesgue measure) by the requirement that if $A \subset S$ is also a support for $d\mu^\theta_{\text{a.c.}}$ then $\text{meas}(S - A) = 0$. Finally, let $f_\pm(x,\theta,E)$ be the solution of

$$L_\theta f = Ef \tag{1.1}$$

with $\text{Im}\, E \neq 0$, $f \in L^2(\mathbb{R}_\pm)$, $\mathbb{R}_+ \equiv (0,\infty)$, $\mathbb{R}_- \equiv (-\infty,0)$. Denoting by d/dE the Radon–Nicodym derivative with respect to Lebesgue measure, by $[g,h]$ the Wronskian $gh' - g'h \equiv g(dh/dx) - (dg/dx)h$ and by (ϕ,f) the L^2 product $\int_{\mathbb{R}} \phi(x)\bar{f}(x)dx$, we have the following theorem.

Theorem 1.1: For any $\phi \in C_0^\infty$, for a.e. $(\theta,E) \in \mathbb{T}^d \times S$,

$$\frac{d\mu^\theta_{\phi,\text{a.c.}}}{dE} = \frac{1}{2\pi i} \frac{|(\phi,f)|^2 + |(\phi,\bar{f})|^2}{[f,\bar{f}]},$$

where $f(x,\theta,E) \equiv \lim_{\epsilon \downarrow 0} f_+(x,\theta,E+i\epsilon)$ and $i[f,\bar{f}] > 0$.

Throughout this paper a fundamental role is played by Bloch waves (or Floquet solutions). These are eigensolutions of the form $\psi = e^{i\beta x}\chi$ with $\beta \in \mathbb{R}$ and χ a quasiperiodic function with basic frequencies ω.

Theorem 1.2: Let $I \subset \mathbb{R}$ be a set of positive Lebesgue measure and assume that for a.e. (θ,E) in $\mathbb{T}^d \times I$ there exists a Bloch wave ψ. Then $I \subset S$, $[\psi,\bar{\psi}] \neq 0$ and, for any $\phi \in C_0^\infty$,

$$\frac{d\mu^\theta_{\phi,\text{a.c.}}}{dE} = \frac{1}{2\pi} \frac{|(\phi,\psi)|^2 + |(\phi,\bar{\psi})|^2}{|[\psi,\bar{\psi}]|},$$

$$(\theta,E) \text{ a.e. in } \mathbb{T}^d \times I.$$

In Ref. 3 Deift and Simon showed that, for a.e. (θ,E) in $\mathbb{T}^d \times S$ there exist eigensolutions $g = e^{i[\alpha x + \beta(x)]}r(x)$, with $[g,\bar{g}] = -2i$ and α being the Johnson–Moser rotation number,[7,10] such that r is an L^2 quasiperiodic function, i.e., $r(x,\theta,E) = R(T_x\theta)$ with $R(\cdot,E) \in L^2(\mathbb{T}^d)$. However, no quasiperiodicity properties were proved for the phase β. Now assume that ω satisfies a Diophantine condition like

$$|\omega \cdot \nu| \equiv \left| \sum_{i=1}^d \omega_i \nu_i \right| \geqslant \frac{1}{c|\nu|^\tau},$$

$$|\nu| \equiv \sum |\nu_i| \quad (\text{any } \nu \in \mathbb{Z}^d - 0, \text{ some } c,\tau > 0), \tag{1.2}$$

and denote by

$$\mathbf{0} \equiv \left\{ \Phi \in C^\infty(\mathbb{T}^d) : \int \Phi = 0 \right\}.$$

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Then β is an (ω) quasiperiodic distribution on 0 in the sense of the following theorem.

Theorem 1.3: There exists a distribution B on $C^\infty(\mathbb{T}^d)$ such that for any $\Phi\in\mathbf{0}$,

$$\langle B,\Phi\rangle = \lim_{x\uparrow\infty}\frac{1}{x}\int_0^x \beta(y,\theta,E)\bar{\Phi}(T_y\theta)dy,$$
$$(\theta,E) \text{ a.e. in } \mathbb{T}^d\times S. \tag{1.3}$$

Remark 1.4: Equation (1.3) determines B uniquely on $\mathbf{0}$. Taking $\Phi = e^{i\nu\cdot\theta}$, (1.3) shows that all the quasiperiodic Fourier coefficients (with $\nu\neq 0$) of β are well defined and are equal to $\hat{B}_\nu e^{i\nu\cdot\theta}$, $\hat{B}_\nu \equiv \langle B, e^{i\nu\cdot\theta}\rangle$.

Remark 1.5: Theorems 1.1 and 1.2 can be trivially extended to the case of almost periodic Schrödinger operators. Theorem 1.3 is false if ω fails to satisfy any Diophantine condition, i.e., if ω is a "Liouville vector"; compare Ref. 1.

The problem of characterizing the a.c. spectrum in terms of genuine Bloch waves remains open but we will see that it is closely related to the analysis of regularity properties of a nonlinear partial differential equation (PDE) on $\mathbb{T}^d$, namely,

$$D_\omega^2 F = \frac{1}{F^3} + (V-E)F, \quad F(\theta)>0 \quad \text{for a.e. } \theta, \tag{1.4}$$

where

$$D_\omega \equiv \sum_{i=1}^d \omega_i \frac{\partial}{\partial\theta_i}.$$

Equation (1.4) will be shown to be satisfied, for a.e. E in S, by $R(\cdot,E)$ in the sense of distributions.

We pass now to the constructive part of the theory. The operators that we shall consider are of the form $L^{(\epsilon)}\equiv L(v+\epsilon w)$, $v+\epsilon w\equiv V(\omega_1 x)+\epsilon W(\omega_2 x,\ldots,\omega_d x)$, with V,W real analytic on, respectively, $\mathbb{T},\mathbb{T}^{d-1}$ and ϵ a positive number. The vector ω is assumed to satisfy a generalized Diophantine condition

$$|\omega\cdot\nu|\geqslant 1/c\Omega(|\nu|), \quad \nu\in\mathbb{Z}^d-0,\ c>0 \quad \text{(fixed)}, \tag{1.5}$$

where $\Omega(r)\geqslant r^{d-1}$ is a monotone function growing not too fast as $r\uparrow\infty$ (see Ref. 9). Then, employing a Kolmogorov–Arnold–Moser (KAM) technique,[11–13] we will construct, for small $c\epsilon/\kappa$, a subset $\mathbf{E}^{(\epsilon)}$ of $\sigma(L^{(0)})\cap\sigma(L^{(\epsilon)})$ and for each $E\in E^{(\epsilon)}$ a Bloch wave $e^{i\alpha x}\chi(\omega x)$ with (α,ω) rationally independent and $\chi(\theta)$ analytic on $\mathbb{T}^d$. The parameter κ is a function of E asymptotic to $\sqrt{E}$ and, for some $a,b>0$ and for any $E_0>0$, the set $\mathbf{E}^{(\epsilon)}$ satisfies

$$\text{meas}\{(\sigma(L^{(0)})-\mathbf{E}^{(\epsilon)})\cap[E_0,\infty)\}$$
$$\leqslant \frac{a}{c}\left(\sum_{|\nu|>bE_0}\frac{|\nu|\log\log\Omega(|\nu|)}{\Omega(|\nu|)}\right). \tag{1.6}$$

The connection with the general part is then given by Theorem 1.2 which yields immediately $\mathbf{E}^{(\epsilon)}\subset\sigma_{\text{a.c.}}(L^{(\epsilon)})$.

Before constructing such Bloch waves we will explain that the existence of quasiperiodic eigenfunctions corresponds to quasiperiodic Hamiltonian flows on $(d+1)$-dimensional tori; see, also, Refs. 14 and 15. In general, to any operator $L_{\theta_0}(u)$, $u(x)\equiv U(T_x\theta_0)$, we can associate the $(d+1)$-dimensional Hamiltonian

$$H_U(p,B,q,\theta;E)\equiv p^2/2+\omega\cdot B+(q^2/2)[E-U(\theta)],$$

where $(p,B)\in\mathbb{R}^{d+1}$ denote the generalized momenta and $(q,\theta)\in\mathbb{R}\times\mathbb{T}^d$ denote the generalized coordinates. It is readily checked that the evolution equation for q [with initial data $q(0),p(0)\equiv q'(0),\theta(0)\equiv\theta_0$] is nothing but the eigenvalue equation $L_{\theta_0}q=Eq$. What we will see is that, for $E\in\mathbf{E}^{(\epsilon)}$, $H_{V+\epsilon W}$ is canonically conjugate to a system of harmonic oscillators with Hamiltonian $\alpha A_0+\omega_1 A_1+\cdots+\omega_d A_d$ in action-angle variables $(A,\theta)\in\mathbb{R}_+\times\mathbb{R}^d\times\mathbb{T}^{d+1}$. This fact, from one side, clarifies the use of KAM techniques in the theory of quasiperiodic Schrödinger operators and, on the other side, gives a rather natural interpretation of spectral quantities such as a.c. eigenfunctions and the rotation number in terms of Hamiltonian objects. Actually we believe that the Hamiltonian H_U is integrable whenever $E\in\sigma_{\text{a.c.}}(L(u))$.

In our treatment of these matters we refine some aspects of the Dinaburg–Sinai–Rüssmann theory. For example, we will see that KAM objects, such as rotation number and Bloch waves constructed on $\mathbf{E}^{(\epsilon)}$ are C^∞ functions of $E\in\mathbf{E}^{(\epsilon)}$ in the sense of Whitney.[16–18] Exploiting this fact it will be easy to give a self-contained and complete description of the KAM spectrum $\mathbf{E}^{(\epsilon)}$ that was still missing in the literature.

Since the basic KAM techniques are by now well known (see, e.g., Ref. 19), most of the proofs in this second part will be outlined without going into detail.

The content of the rest of the paper is the following: Sec. II, proof of Theorem 1.1; Sec. III, Bloch waves; Sec. IV, weak Bloch waves; Sec. V, periodic Schrödinger operators as harmonic oscillators; Sec. VI, quasiperiodic perturbations; Sec. VII, KAM Bloch waves; Sec. VIII, Whitney smoothness; Sec. IX, structure of KAM spectra; Appendix A: on a new condition in analytic KAM; Appendix B: Moser–Deift–Simon inequality on KAM spectra.

II. PROOF OF THEOREM 1.1

We need the following facts:

(a) $$\frac{d\mu_{\phi,\text{a.c.}}}{dE} = \lim_{\epsilon\downarrow 0}\text{Im}(R_{E+i\epsilon}\phi,\phi),$$
$$R_E\equiv(L-E)^{-1},$$

for any $\phi\in C_0^\infty$ and a.e. E in S.

(b) $$R_E(x,y)\equiv g(x,y;E)$$
$$= f_+(x)f_-(y)/[f_+,f_-], \quad \text{Im } E\neq 0,$$

for $x\geqslant y$ and symmetrically for $x<y$ ($f_\pm$ are the eigenfunctions introduced in Sec. I).

(c) $$f_\pm(x,\theta,E) = \text{const}(f_1(x,\theta,E)$$
$$\pm h_\pm(\theta,E)f_2(x,\theta E)),$$

where f_1, f_2 solve (1.1) with $f_1(0)=f_2'(0)=1, f_1'(0)=f_2(0)=0$ and $h_\pm$ are, for every θ, the Herglotz functions defined by $\lim_{x\to\pm\infty}\mp f_1/f_2$. We recall that a function h is Herglotz if it maps holomorphically the open upper half plane $\mathbb{C}_+$ into itself. We will denote the boundary value of h,

existing a.e. on $\mathbb{R}$, by the same symbol. For more information see, e.g., Ref. 20.

(d) For a.e. E in $\mathbb{R}$,

$$-\lim_{\epsilon\downarrow 0}\operatorname{Re}\int_{\mathbb{T}^d} h_+(\theta,E+i\epsilon)d\theta$$
$$\equiv\gamma(E)=\gamma_+(E,\theta)$$
$$\equiv\text{(highest) Lyapunov exponent for } L_\theta - E$$

and

$$S=\{E:\gamma(E)=0\}\subset\{E:h_+=-\bar{h}_-,\ \operatorname{Im}h_+>0\}.$$

Equation (a) is a simple consequence of Stone's formula (see, e.g., Ref. 21). Equations (b) and (c) are the main results of Weyl's limit-point theory (see Ref. 22). Equation (d) is proved in Ref. 2.

Notice that, for a.e. $E, f_\pm(x,\theta,E+i\epsilon)$ converge, as $\epsilon\downarrow 0$, uniformly on compact x sets. Also, for a.e. E in S, (d) shows that $f_+=\bar{f}_-$ with $[f_+,f_-]=-2i\operatorname{Im}h_+$. These observations together with (a) and the evaluation

$$\operatorname{Re}\iint_{x>y}\psi(x)\bar{\psi}(y)\phi(x)\bar{\phi}(y)dx\,dy=\frac{1}{2}|(\bar{\psi},\phi)|^2,$$

valid for any $\psi\in C(\mathbb{R})$ and $\phi\in C_0^\infty(\mathbb{R})$, make Theorem 1.1 plain.

III. BLOCH WAVES

In this section we prove some elementary properties of (genuine≡smooth) Bloch waves and Theorem 1.2.

Lemma 3.1: (i) If $\psi(x)=e^{i\beta x}\chi(\omega x)$ is a Bloch wave for L_0-E then $\psi(x,\theta)\equiv e^{i\beta x}\chi(T_x\theta)$ is a Bloch wave for $L_\theta-E$.

(ii) Let I be as in Theorem 1.2. Then ψ can be written (a.e. on I) in the form $e^{i\alpha x}\chi(T_x\theta)$ with (α,ω) rationally independent.

(iii) If $\psi=e^{i\alpha x}\chi(\omega x)$ is a Bloch wave (α,ω) rationally independent, then $[\psi,\bar{\psi}]\neq 0$ and $\min_{\mathbb{T}^d}|\psi|>0$.

Proof: Since ψ solves (1.1) with $\theta=0$, χ satisfies

$$D_\omega^2\chi+2i\beta D_\omega\chi+(E-\beta^2-V)\chi=0 \tag{3.1}$$

at $\theta=\omega x$. But because $\{\theta=\omega x: x\in\mathbb{R}\}$ is dense in $\mathbb{T}^d$, (3.1) holds identically on $\mathbb{T}^d$. In particular, it holds at $\theta+\omega x$ and (i) is proved.

Property (ii) follows easily from (i) and the fact that $E\in\mathbb{R}\to\alpha(E)\in\overline{\mathbb{R}}_+$ is an increasing function, constant only on spectral gaps where it takes value in $\{\omega\cdot\nu/2,\nu\in\mathbb{Z}^d\}$; see Ref. 7.

If $[\psi,\bar{\psi}]=0$ we would have $\chi=ae^{-2i\alpha x}\bar{\chi}$, for some $a\in\mathbb{C}$. But two quasiperiodic functions cannot be equal unless they have the same basic frequencies; see, e.g., Ref. 23. Thus $[\psi,\bar{\psi}]\neq 0$. If $|\psi|$ were not bounded away from 0, there would exist $x_n\uparrow\infty$ for which $\psi(\omega x_n)\to 0$, but this would imply $[\psi,\bar{\psi}]=0$, a contradiction. □

Proof of Theorem 1.2: From the above lemma $[\psi,\bar{\psi}]\neq 0$ (a.e.) on I. Thus the Lyapunov number vanishes a.e. on I and $I\subset S$ by Kotani's results [see (d), Sec. II]. Now fix E (a.e.) in I and let g be the Deift–Simon function described in Sec. I. Then, for a.e. θ and all x,

$$g(x,\theta)=a\psi(x,\theta)+b\bar{\psi}(x,\theta)$$

for some complex numbers a,b depending on θ. Taking absolute values one obtains

$$R^2(T_x\theta)+c|\chi(T_x\theta)|^2$$
$$=de^{2i\alpha x}\chi^2(T_x\theta)+\bar{d}e^{-2i\alpha x}\bar{\chi}^2(T_x\theta),$$

where $c=-(|a|^2+|b|^2)$ and $d=2a\bar{b}$. Now take $y>0$ and $\nu\in\mathbb{Z}^d$. Multiply the above equation by $(1/y)\exp[-2i(t+\alpha x)-iT_x\theta\cdot\nu]$ and integrate it from 0 to y with respect to x. Since R^2 and $|\chi|^2$ belong to $L^1(\mathbb{T}^d)$ we can use the ergodic theorem to let $y\uparrow\infty$ and conclude

$$0=de^{-2it}(\hat{\chi}^2)_\nu,\ \text{for all } \nu,\ \text{a.e. } (t,\theta)\in\mathbb{T}^{d+1},$$

where $(\hat{\ })_\nu$ denote Fourier coefficients. This shows that $d=0$, i.e., either $a=0$ or $b=0$. Theorem 1.2 follows now from Theorem 1.1. □

IV. WEAK BLOCH WAVES

Here we discuss the a.c. Deift–Simon eigenfunctions g on S and prove Theorem 1.3. Henceforth we will often omit the sentence (E,θ) a.e. in $S\times\mathbb{T}^d$.

Since $[g,\bar{g}]=-2i$, $r(x)$ never vanishes and the normalized phase β is a well-defined function from $\mathbb{R}\to\mathbb{R}$. The Schrödinger equation for g implies

$$r''=1/r^3+(v_\theta-E)r, \tag{4.1}$$
$$\beta'=1/r^2-\alpha, \tag{4.2}$$

with initial data $r(0)=R(\theta)$, $r'(0)=D_\omega R(\theta)$, and $\beta(0)=0\ (\mathrm{mod}\ 2\pi)$. [The initial value for β is explained by the identification $g(x,\theta,E)=R(\theta)f(x,\theta,E)$, cf. Ref. 3]. Deift and Simon in Ref. 3, extending to S a formula by Johnson and Moser, proved

$$\lim_{x\uparrow\infty}\frac{1}{x}\int_0^x\frac{1}{r^2}=\int_{\mathbb{T}^d}\frac{1}{R^2}=\alpha. \tag{4.3}$$

This, together with the Schrödinger equation for g, yields easily the finiteness of

$$\overline{\lim}\,\frac{1}{x}\int_0^x|g'|^2\ \text{and}\ \overline{\lim}\,\frac{|r'|+r+r^{-1}}{x}. \tag{4.4}$$

Our next goal is to show that (4.1) and (4.3) imply $R^{-3}\in L^1$ and that R is a distributional solution of (1.4). Let $0\leqslant\Phi\in C^\infty(\mathbb{T}^d)$ and write $\phi(x)=\phi(x,\theta)\equiv\Phi(T_x\theta)$. Then by the ergodic theorem, (4.4) and (4.1),

$$\int_{\mathbb{T}^d}RD_\omega^2\phi=\lim_{x\uparrow\infty}\frac{1}{x}\int_0^x R(T_y\theta)(D_\omega^2\Phi)(T_y\theta)dy$$
$$=\lim\frac{1}{x}\int_0^x r\phi''$$
$$=\lim\frac{1}{x}\left\{[r\phi']_0^x-[r'\phi]_0^x+\int_0^x r''\phi\right\}$$
$$=\lim\frac{1}{x}\int_0^x\left(\frac{1}{r^3}+(v_\theta-E)r\right)\phi. \tag{4.5}$$

Another application of the ergodic theorem to positive random variables shows

$$\lim \frac{1}{x}\int_0^x \frac{\phi}{r^3} = \int_{\mathbb{T}^d} \frac{\Phi}{R^3}.$$

But then from (4.5) we conclude, *a fortiori*, that

$$\int_{\mathbb{T}^d} \frac{\Phi}{R^3} = \int_{\mathbb{T}^d} (E-V)R\Phi + \int_{\mathbb{T}^d} RD_\omega^2\,\Phi < \infty. \tag{4.6}$$

In particular, by taking $\Phi \equiv 1$ we get

$$\int_{\mathbb{T}^d} \frac{1}{R^3} = \int_{\mathbb{T}^d} (E-V)R. \tag{4.7}$$

Now we can repeat the computation in (4.5) with an arbitrary $\Phi \in C^\infty(\mathbb{T}^d)$ and get back (4.6). This is the same as saying the R is a weak solution of (1.4).

Next we turn to the proof of Theorem 1.3. Since ω satisfies (1.2),

$$B(\theta) \equiv \sum_{\nu\neq 0} \frac{1}{i\omega\cdot\nu}\left(\frac{\hat{1}}{R^2}\right)_\nu e^{i\nu\cdot\theta}$$

is seen to be a distribution on $C^\infty(\mathbb{T}^d)$. In fact, if $t > \tau + d/2$,

$$\begin{aligned}
&\sum_{\nu\neq 0} |\hat{B}_\nu|^2 (1+\nu\cdot\nu)^t \\
&\quad \equiv \sum_{\nu\neq 0} \frac{1}{|\omega\cdot\nu|^2}\left|\left(\frac{\hat{1}}{R^2}\right)_\nu\right|^2 \frac{1}{(1+\nu\cdot\nu)^t} \\
&\quad < c^2\left(\int \frac{1}{R^2}\right)^2 \sum \frac{|\nu|^{2m}}{(1+\nu\cdot\nu)^t} < \infty
\end{aligned}$$

shows that $B \in H_{-t}(\mathbb{T}^d)$. Now denote by D_ω^{-1} the linear operator

$$D_\omega^{-1}: \Phi \in \mathbf{0} \to D_\omega^{-1}\Phi \equiv \sum_{\nu\neq 0} \frac{\hat{\Phi}_\nu}{i\omega\cdot\nu} e^{i\nu\cdot\theta} \in \mathbf{0}.$$

Then by (4.3), the ergodic theorem, and (4.2) we have

$$\begin{aligned}
\langle B,\Phi\rangle &= \langle B, D_\omega D_\omega^{-1}\Phi\rangle \\
&= -\langle D_\omega B, D_\omega^{-1}\Phi\rangle \\
&= -\langle 1/R^2 - \alpha, D_\omega^{-1}\Phi\rangle \\
&\equiv -\int \left(\frac{1}{R^2}-\alpha\right)\overline{D_\omega^{-1}\Phi} \\
&= -\lim \frac{1}{x}\int_0^x \left(\frac{1}{R^2}-\alpha\right)\overline{D_\omega^{-1}\Phi}(T_y\theta)\,dy \\
&= -\lim \frac{1}{x}\int_0^x \beta'\,\overline{D_\omega^{-1}\Phi}(T_y\theta)\,dy \\
&= -\lim \frac{1}{x}\left[\beta\,\overline{D_\omega^{-1}\Phi}(T_y\theta)\right]_0^x \\
&\quad + \lim \frac{1}{x}\int_0^x \beta\bar{\Phi}(T_y\theta) \\
&= \lim \frac{1}{x}\int_0^x \beta\bar{\Phi}(T_y\theta),
\end{aligned}$$

in which the last equality holds because α is the rotation number of g so that $\lim(1/x)\,\beta(x) = 0$. □

To connect the existence of smooth Bloch waves with regularity properties for (1.4), assume that V is of class $C^\infty(\mathbb{T}^d)$ and that R is a smooth solution of (1.4). Then, by the equation, $\min R > 0$ and $1/R^2 - \alpha$ belongs to $C^\infty(\mathbb{T}^d)$. Thus also B, as defined above, is a smooth function and we can identify $\beta(x,\theta)$ with the quasiperiodic solution of (4.2) $B(T_x\theta) - B(\theta)$. Unfortunately, regularity properties for such nonlinear equations on tori are difficult to obtain by general PDE methods. (See, however, Ref. 24.)

V. PERIODIC SCHRÖDINGER OPERATORS AS HARMONIC OSCILLATORS

From now on we will be concerned with the constructive part of the theory. In this section we look at periodic Schrödinger operators $L^{(0)}$ from the Hamiltonian point of view described in the Introduction. We show briefly that for each E in the interior $\overset{0}{\sigma}$ of the spectrum σ of $L^{(0)}$, the Hamiltonian H_V of Sec. I is conjugated to $\alpha_0 A_0 + \omega_1 A_1$, $(A_0,A_1) \in \mathbb{R}_+ \times \mathbb{R}$, $\alpha_0 \equiv$ rotation number for $L^{(0)} - E$. (We learned about the integrability of H_V in Ref. 15.) For more details on this and the following sections see Ref. 25.

From Floquet theory[26] one knows that, for each $E \in \overset{0}{\sigma}$, there exist two independent Bloch waves $f_0, \bar{f}_0$ of the form

$$\begin{aligned}
f_0(x) &\equiv e^{i\alpha_0 x}\chi_0(\omega_1 x) \\
&\equiv f_1(x) + \frac{e^{i\alpha_0(2\pi/\omega_1)} - f_1(2\pi/\omega_1)}{f_2(2\pi/\omega_1)} f_2(x), \\
&\quad \chi_0 \in C(\mathbb{T}),
\end{aligned}$$

with

$$\kappa \equiv \frac{i}{2}[f_0,\bar{f}_0] = \operatorname{Im} f_0'(0) = \frac{\sin(\alpha_0(2\pi/\omega_1))}{f_2(2\pi/\omega_1)} > 0.$$

Now define

$$Q(\theta_0,\theta_1) \equiv \operatorname{Re} F_0(\theta_0,\theta_1), \quad P(\theta_0,\theta_1) \equiv \operatorname{Re} DF_0(\theta_0,\theta_1),$$

where

$$F_0(\theta_0,\theta_1) \equiv e^{i(\theta_0 - (\alpha_0/\omega_1)\theta_1)} f_0(\theta_1/\omega_1), \quad (\theta_0,\theta_1) \in \mathbb{T}^2,$$

$$D \equiv \alpha_0 \frac{\partial}{\partial\theta_0} + \omega_1 \frac{\partial}{\partial\theta_1}.$$

One recognizes easily that $x \to F_0(\theta_0 + \alpha_0 x, \theta_1 + \omega_1 x)$ is an eigensolution for $L(v_{\theta_1})$ and that

$$\frac{d}{dx} F_0(\theta_0 + \alpha_0 x, \theta_1 + \omega_1 x) = DF_0(\theta_0 + \alpha_0 x, \theta_1 + \omega_1 x).$$

Moreover, from

$$\frac{\partial Q}{\partial\theta_0} P - Q\frac{\partial P}{\partial\theta_0} = \frac{i}{2}[f,\bar{f}] = \frac{i}{2}[f_0,\bar{f}_0] = \kappa > 0,$$

it follows readily that the map

$$\begin{aligned}
&(r,B,\theta_0,\theta_1) \in \mathbb{R}_+ \times \mathbb{R} \times \mathbb{T}^2 \to (p,B,q,\theta_1) \\
&\quad \equiv (rP(\theta_0,\theta_1), B, rQ(\theta_0,\theta_1), \theta_1)
\end{aligned}$$

is a diffeomorphism onto the phase space of H_V, i.e., $\mathbb{R}^3 \times \mathbb{T} - (0,\mathbb{R},0,\mathbb{T})$. Now we can construct a diffeomorphism

$$\mathbf{C}: (p,B,q,\theta_1) \to (A_0,A_1,\theta_0,\theta_1) \in \mathbb{R}_+ \times \mathbb{R} \times \mathbb{T}^2$$

by setting $A_0 = (r^2/2)\kappa$,

$$A_1 = B + \frac{r^2}{2}\left(\frac{\partial Q}{\partial\theta_1} P - Q\frac{\partial P}{\partial\theta_1}\right).$$

Straightforward computations will show first that $dp\wedge dq + dB\wedge d\theta_1 = dA_0\wedge d\theta_0 + dA_1\wedge d\theta_1$, so that C is canonical, and then

$$(p^2/2) + \omega_1 B + (q^2/2)(E - V) = \alpha_0 A_0 + \alpha_1 A_1,$$

confirming what we claimed above.

Remark 5.1: Even for V merely continuous, α_0, f_1, f_2, and κ are real analytic functions of E.[26] Furthermore, α_0 maps $\sigma(L^{(0)})$ onto $[0,\infty)$, $d\alpha_0/dE > 0$ on $\overset{0}{\sigma}$ and, setting $\partial\overset{0}{\sigma} \equiv \{E_0^0 < E_1^0 < \cdots\}$, $a_k^0 \equiv \alpha_0(E_k^0) = h\omega_1/2$ for some integer h. Now denoting by $e_0(a)$, $a\in R_+$, $a\neq a_k^0$, the inverse function of α_0, one can easily show that, if $\rho < \omega_1/4$, e_0 admits a holomorphic extension to

$$D(\rho;\mathbf{A}_0) \equiv \bigcup_{a_0\in\mathbf{A}_0} \{a\in\mathbb{C}: |a - a_0| < \rho\},$$

with

$$\mathbf{A}_0 \equiv \bigcup_{k=0}^{\infty} [a_k^0 + \rho, a_{k+1}^0 - \rho].$$

This will be of later use.

VI. QUASIPERIODIC PERTURBATIONS

Now let $\epsilon > 0$. Under the canonical transformation

$$(p,B_1,\ldots,B_d,q,\theta_1,\ldots,\theta_d)\in\mathbb{R}^{d+2}\times\mathbb{T}^d - (0,\mathbb{R}^d,0,\mathbb{T}^d) \to (A,\theta)$$
$$\equiv (A_0,A_1,\ldots,A_d,\theta_0,\theta_1,\ldots,\theta_d)\in\mathbf{M}\equiv\mathbb{R}_+\times\mathbb{R}^d\times\mathbb{T}^{d+1},$$
$$(A_0,A_1,\theta_0,\theta_1)\equiv\mathbf{C}(p,B,q,\theta_1), \quad A_i = B_i, \quad i\geqslant 2$$

(C as in Sec. V), the Hamiltonian $H_{V+\epsilon W}(\cdot;E)$, $E\in\overset{0}{\sigma}(L^{(0)})$, takes the form

$$H_\epsilon(A,\theta;E) \equiv \omega^{(0)}\cdot A + \epsilon A_0 F(\theta)$$

with

$$\omega^{(0)} \equiv (\alpha_0,\omega), F(\theta) \equiv -[Q^2(\theta_0,\theta_1)/\kappa] W(\theta_2,\ldots,\theta_d).$$

In this section we describe an iterative scheme that will allow us to integrate H_ϵ for special values of the parameter E and small ϵ. Henceforth, it will be more convenient to consider H_ϵ parametrized by the rotation number $\alpha_0 \equiv a$ rather than by the eigenvalue E. It will be only later that we shall express our result directly in terms of eigenvalues. We start by considering the jth order analog of H_ϵ. Let $j\geqslant 0$ and, for $(A,\theta)\in\mathbf{M}$, let

$$H^{(j)}(A,\theta;a,\epsilon) \equiv \omega^{(j)}(a;\epsilon)\cdot A + \epsilon^{2^j} A_0 F^{(j)}(\theta;a,\epsilon),$$
$$\omega^{(j)} \equiv (\omega_0^{(j)},\omega_1,\ldots,\omega_d).$$

Assume that $\omega_0^{(j)}$ and $F^{(j)}$, as functions of a, are holomorphic in

$$D_j \equiv D(\rho_j;\mathbf{A}^{(j)}) \equiv \bigcup_{a_0\in\mathbf{A}^{(j)}} \{a\in\mathbb{C}: |a - a_0| \leqslant \rho_j\}$$

for some $\mathbf{A}^{(j)}\subset\mathbb{R}$. Also, as a function of $\theta\in\mathbb{R}^{d+1}$, $F^{(j)}$ is required to have holomorphic extension to

$$S_j \equiv S^{d+1}(\xi_j) \equiv \{\theta\in\mathbb{C}^{d+1}: |\operatorname{Im}\theta_i| \leqslant \xi_j\}, \quad \xi_j > 0,$$

with

$$\|F^{(j)}\|_{\xi_j,\rho_j} \equiv \sup_{(\theta,a)\in S_j\times D_j} |F^{(j)}| \leqslant M_j$$

independently of ϵ. Notice that because of the analyticity assumptions on V and W, $H_\epsilon(A,\theta;e_0(a))$, $\mathbf{A}_0$ as in Remark 5.1, satisfies the above hypothesis, thus we can set $H^{(0)} \equiv H_\epsilon$. Now, let $\delta_j < \xi_j/2$ and let us define the main recursive objects

$$\zeta(s) \equiv 1 + \sum_{\nu\in\mathbb{Z}^{d+1}-0} |\nu|\Omega(|\nu|)e^{-s|\nu|}, \quad s > 0,$$
$$N_j \equiv 2^{j+1}\delta_j^{-1}\log\epsilon^{-1},$$
$$F_R^{(j)}(\theta) \equiv \sum_{|\nu|>N_j} \hat{F}_\nu^{(j)} e^{i\nu\cdot\theta},$$
$$\rho_{j+1} \equiv \min\left\{\left(2cN_j\Omega(N_j)\sup_{a\in D_j}\left|\frac{d\omega_0^{(j)}}{da}\right|\right)^{-1}, \frac{\rho_j}{2}\right\},$$
$$\xi_{j+1} \equiv \xi_j - 2\delta_j,$$
$$A^{(j+1)} \equiv \{a\in\mathbf{A}^{(j)}: |\omega^{(j)}(a)\cdot\nu| \geqslant 1/c\Omega(|\nu|),$$
$$\nu\in\mathbb{Z}^{d+1} - 0, \ |\nu| \leqslant N_j\},$$
$$D_{j+1} \equiv D(\rho_{j+1};\mathbf{A}^{(j+1)}),$$
$$S_{j+1} \equiv S^{d+1}(\xi_{j+1}).$$

Lemma 6.1 (Inductive Lemma): If $a\in\mathbf{A}^{(j+1)}$ and ϵ is small enough, i.e.,

$$K_1\zeta(\delta_j)\delta_j^{-1} cM_j\epsilon^{2^j} \leqslant 1, \tag{6.1}$$

where K_1 is a universal constant, then the function

$$(A',\theta)\in\mathbf{M}\to A'\cdot\theta + \epsilon^{2^j}A_0\Phi_j(\theta;a,\epsilon),$$
$$\Phi_j \equiv \sum_{0<|\nu|<N_j} \frac{\hat{F}_\nu^{(j)}}{-i\omega^{(j)}\cdot\nu} e^{i\nu\cdot\theta}$$

is the generating function of a surjective canonical transformation, $(A,\theta)\to(A',\theta') = (A'(A,\theta),\theta'(\theta))$, that conjugates $H^{(j)}(A,\theta)$ to

$$H^{(j+1)}(A',\theta';a,\epsilon)$$
$$\equiv H^{(j)}(A(A',\theta'),\theta(\theta'))$$
$$= \omega^{(j+1)}\cdot A' + \epsilon^{2^{j+1}} A_0' F^{(j+1)}(\theta';a,\epsilon),$$

where

$$\omega^{(j+1)} \equiv (\omega_0^{(j)} + \epsilon^{2^j}\hat{F}_0^{(j)},\omega),$$
$$F^{(j+1)}(\theta'(\theta)) \equiv \frac{\partial\Phi_j}{\partial\theta_0}(\theta)F^{(j)}(\theta) + \frac{F_R^{(j)}(\theta)}{\epsilon^{2^j}}.$$

Furthermore, $a\in\mathbf{A}^{(j+1)}\to\omega_0^{(j)}(a)$ and $(\theta,a)\in R^{d+1}\times\mathbf{A}^{(j+1)}\to F^{(j+1)}(\theta;a)$ have holomorphic extensions to, respectively, D_{j+1} and $S_{j+1}\times D_{j+1}$ with

$$\|F^{(j+1)}\|_{\xi_{j+1},\rho_{j+1}} \leqslant K_2\zeta(\delta_j)\delta_j^{-(d+1)} c M_j^2 \equiv M_{j+1}, \tag{6.2}$$

in which K_2 is a second universal constant.

Applying this Lemma infinitely many times one can integrate H_ϵ for $a\in\mathbf{A}^{(\infty)} \equiv \cap_{j=0}^{\infty}\mathbf{A}^{(j)}$.

Theorem 6.2: Let $\{\delta_j\}$ be such that $\Sigma_{j=0}^{\infty}\delta_j < \xi/2$, let $a\in\mathbf{A}^{(\infty)}$ and let ϵ verify

$$(K_1/K_2)\epsilon\tau \leqslant 1 \tag{6.3}$$

with

$$\tau \equiv K_2\psi cM_0, \quad \psi \equiv \prod_{j=0}^{\infty}[\zeta(\delta_j)\delta_j^{-(d+1)}]^{1/2^j}.$$

Then the Hamiltonian $H^{(0)}$ is conjugate to

$$H^{(\infty)} \equiv \omega^{(\infty)} \cdot A,$$

where $\omega^{(\infty)} \equiv (\omega_0^{(\infty)}, \omega)$ satisfies

$$\begin{aligned} &c|\omega_0^{(\infty)} - a| \leqslant \frac{1}{K_2} \sum_{j=0}^{\infty} (\epsilon\tau)^{2^j}, \\ &|\omega^{(\infty)} \cdot \nu| \geqslant \frac{1}{c\Omega(|\nu|)}, \quad \nu \in \mathbb{Z}^{d+1} - 0. \end{aligned} \tag{6.4}$$

The (surjective) canonical transformation conjugating $H^{(0)}$ to $H^{(\infty)}$ has the form

$$\begin{aligned} &(A', \theta') \in \mathbf{M} \to (A, \theta) \\ &\quad \equiv (S(\theta')A', \theta_0' + \epsilon\Delta(\theta_0'), \theta_1', \ldots, \theta_d') \in \mathbf{M} \end{aligned} \tag{6.5}$$

with S a $(d+1) \times (d+1)$ matrix of the form

$$\begin{bmatrix} 1 + \epsilon s_0 & 0 & 0 & \cdots & 0 \\ \epsilon s_1 & 1 & 0 & \cdots & 0 \\ \vdots & & & & \\ \epsilon s_d & 0 & 0 & \cdots & 1 \end{bmatrix}.$$

Moreover, the vector $s \equiv (s_0, \ldots, s_d)$ and Δ have holomorphic extensions to $S^{d+1}(\xi_\infty)$, $\xi_\infty \equiv \xi - 2\sum_{j=0}^{\infty} \delta_j$, and

$$\max\{\|s\|_{\xi_\infty}, \|\Delta\|_{\xi_\infty}\} \leqslant (K_1/K_2)\tau.$$

Remark 6.3: Examples of $\{\delta_j\}$ and Ω such that $\psi < \infty$ are displayed in Appendix A.

Remark 6.4: Perturbations of the Hamiltonian of the form $h(A, \theta) \equiv \tilde{\omega} \cdot A$ were investigated in Refs. 27 and 28 using Moser's idea of "modified systems."[29]

Remark 6.5: An easy corollary of Theorem 6.2 is that all the eigensolutions of $L^{(\epsilon)}$ for $E \in \tilde{\mathbf{E}}^{(\epsilon)} \equiv \alpha_0^{-1}(\mathbf{A}^{(\infty)})$ are quasiperiodic with basic frequencies $(\omega_0^{(\infty)}, \omega)$. Also, since all the transformations involved in the process are close to the identity it is easy to see that $\omega_0^{(\infty)}$ coincides with the rotation number α.

Remark 6.6: From an elementary asymptotic analysis ($E \gg 1$) of the periodic case, one realizes that $\|Q^2\|/K \sim 1/\sqrt{E}$ so that $M_0 \sim \|W\|/\sqrt{E}$.

VII. KAM BLOCH WAVES

Even though we already obtained a complete description of the quasiperiodic eigenfunctions of $L^{(\epsilon)}$ for $E \in \tilde{\mathbf{E}}^{(\epsilon)}$, it is not immediate from the above analysis that such eigenfunctions are of the form $e^{i\alpha x}\chi(\omega x)$. Since this representation is crucial in the application of Theorem 1.2, we proceed now with a direct construction of Bloch waves for values of E in a set $\mathbf{E}^{(\epsilon)} \subset \sigma(L^{(0)})$, which *a priori* need not be identical to $\tilde{\mathbf{E}}^{(\epsilon)}$.

The eigenvalue equation $L^{(\epsilon)} f = Ef$ is equivalent to the first-order system

$$\begin{aligned} &y' = \begin{bmatrix} 0 & 1 \\ V(\theta_1) - E & 0 \end{bmatrix} y + \epsilon W(\theta_2, \ldots, \theta_d) \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix} y, \\ &\theta' = \omega, \end{aligned} \tag{7.1}$$

with $y = \begin{pmatrix} f \\ f' \end{pmatrix}$. A fundamental matrix for (7.1) at $\epsilon = 0$ is

$$Y = \begin{bmatrix} f_0 & \bar{f}_0 \\ f_0' & \bar{f}_0' \end{bmatrix} \quad (f_0 \text{ as in Sec. V}).$$

By setting

$$Y = Te^{Cx}, \quad T \equiv \begin{bmatrix} \chi_0(\omega_1 x) & \bar{\chi}_0 \\ i\alpha_0\chi_0 + \omega_1\chi_0' & -i\alpha_0\bar{\chi}_0 + \omega_1\bar{\chi}_0' \end{bmatrix},$$

$$C \equiv \begin{bmatrix} i\alpha_0 & 0 \\ 0 & -i\alpha_0 \end{bmatrix},$$

the system (7.1) becomes, under the change of variable $y = Tz$,

$$z' = Cz + \epsilon Pz, \quad \theta' = \omega \tag{7.2}$$

with

$$P \equiv \frac{W(\theta_2, \ldots, \theta_d)}{2\kappa} \begin{bmatrix} -i|\chi_0(\theta_1)|^2 & -i\bar{\chi}_0^2(\theta_1) \\ i\chi_0^2 & i|\chi_0|^2 \end{bmatrix}.$$

Notice that $P \in \mathbf{G}_0 \equiv \{G \in \mathbf{G}: \operatorname{tr} \int_{\mathbb{T}^d} G = 0\}$ where $\mathbf{G}$ denotes the ring of matrix-valued functions on $\mathbb{T}^d$ of the form

$$G = \begin{bmatrix} g & h \\ \bar{h} & \bar{g} \end{bmatrix}.$$

Theorem 7.1: If ϵ satisfies the smallness condition

$$(K_1/K_2)\epsilon\tau \leqslant 1, \quad \tau \equiv K_2 \psi c M_0,$$

where K_1 and K_2 are suitable universal constants, then one can construct a set $\mathbf{E}^{(\epsilon)} \subset \sigma(L^{(0)})$ and, for each $E \in \mathbf{E}^{(\epsilon)}$, a change of variables $z = (I + \epsilon U)w$, with $U \in G_0$, which transforms (7.2) into the trivial system

$$w' = \begin{bmatrix} i\alpha & 0 \\ 0 & -i\alpha \end{bmatrix} w, \quad \theta' = \omega.$$

Furthermore, U as a function of $\theta \in \mathbf{T}^d$ admits a holomorphic extension to $S^d(\xi_\infty)$, for a suitable $\xi_\infty > 0$, with $\|U\|_{\xi_\infty} \leqslant (K_1/K_2)\tau$ and α verifies

$$\begin{aligned} &|\alpha - |\omega \cdot \nu/2|| \geqslant \frac{1}{c\Omega(|\nu|)}, \quad \nu \in \mathbb{Z}^d - 0, \quad E \in \mathbf{E}^{(\epsilon)}, \\ &\sup_{E \in \mathbf{E}^{(\epsilon)}} |\alpha - \alpha_0| < \epsilon\tau/c. \end{aligned}$$

Remark 7.2: Above we used the same symbols for quantities that are analogous, but not always identical, to the ones appearing in Sec. VI.

The proof of this result is based on a scheme very similar to the one described in Sec. VI: One removes infinitely many times the order of the perturbation of systems like

$$z_j' = \begin{bmatrix} i\alpha_j & 0 \\ 0 & -i\alpha_j \end{bmatrix} z_j + \epsilon^{2^j} P^{(j)} z_j, \quad \theta' = \omega \quad (P^{(j)} \in \mathbf{G}_0),$$

by the aid of a change of variable $(I + \epsilon^{2^j} U_j(\theta))z_{j+1} = z_j$. The set $\mathbf{E}^{(\epsilon)}$ will be given by $\alpha_0^{-1}(\mathbf{A}^{(\infty)})$ where $\mathbf{A}^{(\infty)} \equiv \cap \mathbf{A}^{(j)}$, where as in Sec. V, $\mathbf{A}^{(0)}$ is the positive half-line minus suitable intervals of length 2ρ and

$$\begin{aligned} \mathbf{A}^{(j+1)} \equiv \{&a \in \mathbf{A}^{(j)}: |\alpha_j(a) - \omega \cdot \nu/2| \geqslant 1/c\Omega(|\nu|), \\ &\nu \in \mathbb{Z}^d, \ 0 < |\nu| \leqslant N_j\} \end{aligned}$$

with N_j denoting the jth cutoff in the Fourier expansion of $P^{(j)}$.

VIII. WHITNEY SMOOTHNESS

In this section we study the E dependence of the KAM limits. Following Ref. 16 we say that a function f: $\mathbf{A} \subset \mathbb{R} \to \mathbb{R}$ belongs to $C_W^n(\mathbf{A})$ if there exist, on $\mathbf{A}$, functions f_k, $0 \leqslant k \leqslant n$,

$f_0 \equiv f$, with the following property: For each $x_0 \in A$ and $\epsilon > 0$ there is a $\delta > 0$ s.t. if $x, x' \in \{y \in \mathbf{A}: |y - x_0| < \delta\}$ then

$$\left| f_k(x) - \sum_{h=0}^{n-k} \frac{f_{h+k}(x')}{h!}(x - x')^h \right| \leqslant \epsilon |x - x'|^{n-k}. \quad (8.1)$$

At interior points this definition coincides with the standard one but the next lemma shows how nontrivial $C^n_W(\mathbf{A})$ functions can arise.

Lemma 8.1: Let $\mathbf{A} \subset \mathbb{R}$, $r_j \downarrow 0$, and $\{g_j\}$ be a sequence of holomorphic functions on $D(r_j, \mathbf{A})$ which are real on $\mathbf{A}$. If

$$\sum \|g_j\|_{r_j} r_j^{-n} < \infty,$$

then $g \equiv \Sigma g_j$ belongs to $C^n_W(\mathbf{A})$.

Proof: Since for any $k \leqslant n$

$$\sup_{\mathbf{A}} \left| \frac{d^k g}{dx^k} \right| \leqslant \sum \left| \left| \frac{d^k g_j}{dx^k} \right| \right|_{r_j/2} \leqslant 2^k \sum \|g_j\|_{r_j} r_j^{-k} < \infty,$$

we can define

$$\frac{d^k g}{dx^k} \equiv \sum \frac{d^k g_j}{dx^k}$$

on A. To check that the $d^k g/dx^k$ are the Whitney derivatives of g, let x, $x' \in \mathbf{A}$, let $s = s(|x - x'|)$ be such that $r_{s+1} \leqslant |x - x'| < r_s$, and consider the splitting $g = g^{[s]} + \tilde{g}^{[s]}$ with $g^{[s]} \equiv \Sigma^s g_j$. The lemma follows now from $g^{[s]} \in C^\infty \times (D(r_s; \mathbf{A}) \cap \mathbf{R})$, the inequality

$$\sup_{\mathbf{A}} \left| \frac{d^k \tilde{g}^{[s]}}{dx^k} \right| \leqslant 2^n \sum_{j=s+1}^{\infty} \|g_j\|_{r_j} r_j^{-n}$$

and from $\lim_{|x-x'| \downarrow 0} s(|x - x'|) = \infty$. □

The KAM limits of Secs. VI and VII are exactly of the above kind. For example,

$$\omega_0^{(\infty)} = a + \sum_0^\infty \epsilon^{2^j} \hat{F}_0^{(j)}(a),$$

with $\hat{F}_0^{(j)}$ holomorphic on $D(\rho_j; \mathbf{A}^{(\infty)})$ and one has the following theorem.

Theorem 8.2: If Ω and $\{\delta_j\}$ are such that

$$\prod_{j=0}^{\infty} \zeta(\delta_j)^{1/2^j} < \infty, \quad (8.2)$$

$$\lim_{j \uparrow \infty} \frac{\log \Omega(2^j \delta_j^{-1})}{2^j} = 0, \quad (8.3)$$

and

$$2\left[\epsilon M_0 \rho_0^{-1} + (\epsilon\tau)^2 \sum_{j=0}^{\infty} (\epsilon\tau)^{2^j} N_j \Omega(N_j) \right] < 1, \quad (8.4)$$

then $\omega_0^{(\infty)} \in C^\infty_W(\mathbf{A}^{(\infty)})$.

The proof follows easily after noticing that (8.4) yields

$$\sup_{D(\rho_{j+1}; \mathbf{A}^{(j-1)})} \left| \frac{d\omega_0^{(j)}}{da} - 1 \right| < \frac{2}{3}, \quad (8.5)$$

so that

$$\rho_j^{-1} < 4 N_{j-1} \Omega(N_{j-1}) c. \quad (8.6)$$

For more details see Ref. 25, Sec. 2.6.

Remark 8.3: Whitney smoothness is obviously preserved under composition with smooth functions. Thus $\omega_0^{(\infty)}(\alpha_0(E))$ $(= \alpha(E))$ belongs to $C^\infty_W(\tilde{\mathbf{E}}^{(\epsilon)})$, $\tilde{\mathbf{E}}^{(\epsilon)} \equiv \alpha_0^{-1}(\mathbf{A}^{(\infty)})$.

Remark 8.4: While a condition analogous to (8.2) appears in the (analytic) KAM literature,[8] condition (8.3) is new. This condition is necessary in order to be able to meet the smallness condition (8.4) and, as we shall see, to give a complete description of $\mathbf{A}^{(\infty)}$. We also point out that (8.2) and (8.3) are independent (see Appendix A).

IX. STRUCTURE OF KAM SPECTRA

The main theorem in Ref. 16 is that any function $g \in C^n_W(A)$, $\mathbf{A}$ closed, can be extended to a $C^n(\mathbb{R})$ function which is real analytic on $\mathbb{R} - \mathbf{A}$; a simple corollary of this and of the maximum principle imply

$$\sup_{R} \left| \frac{d^k g}{dx^k} \right| \leqslant \max_{\mathbf{A}} \left| \frac{d^k g}{dx^k} \right|, \quad k \leqslant n.$$

Here we show how to use the above facts in order to give a precise description of the KAM spectrum $\mathbf{E}^{(\epsilon)}$.

Denote by $\mathbf{R}$ the "resonant" set of $a = \alpha_0(E)$ for which we cannot apply the KAM scheme,

$$\mathbf{R} \equiv \mathbf{A}^{(0)} - \mathbf{A}^{(\infty)} \equiv \bigcup_{j=0}^{\infty} \bigcup_{\substack{\nu \in \mathbb{Z}^d \\ 0 < |\nu| < N_j}} \mathbf{R}_\nu^{(j)},$$

where for $0 < |\nu| \leqslant N_j$,

$$\mathbf{R}_\nu^{(j)} \equiv \{a \in \mathbf{A}^{(j)}: |\alpha_j(a) - \omega \cdot \nu/2| < 1/c\Omega(|\nu|)\}.$$

A condition analogous to (8.4) implies easily that the Whitney extension of the α_j's satisfy

$$\sup_{R} \left| \frac{d\alpha_j}{da} - 1 \right| \leqslant \frac{2}{3}.$$

Thus defining

$$a_{j,\nu} \equiv \alpha_j^{-1}(\omega \cdot \nu/2), \quad r_\nu \equiv 3/c\Omega(|\nu|),$$

we see that

$$\mathbf{R}_\nu^{(j)} \subset I_\nu^{(j)} \equiv \{a \in \mathbf{A}^{(0)}: |a - a_{j,\nu}| < r_\nu\}.$$

This completes the description of $\mathbf{A}^{(\infty)}$ and hence, via the smooth map α_0^{-1}, of $\mathbf{E}^{(\epsilon)}$.

Finally it is not difficult to show that[25]

$$\bigcup_{j=0}^{\infty} I_\nu^{(j)} \subset \{|a - a_\nu| < r'_\nu\}, \quad r'_\nu \equiv \frac{7 + \log\log 3\Omega(|\nu|)}{c\Omega(|\nu|)}$$

and $a_\nu \sim \omega \cdot \nu/2$. These facts together with the asymptotic evaluation $\alpha_0(E) \sim \sqrt{E}$ yields (1.4).

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APPENDIX A: ON A NEW CONDITION IN ANALYTIC KAM

Here we show that conditions (8.2) and (8.3) are independent as announced in Remark 8.4. To do this we give two examples.

(1) Let $\Omega(r) = r^m$ for some m. Then

$$(8.2) \Leftrightarrow \sum \frac{1}{2^j} \log \delta_j^{-1} < \infty,$$

$$(8.3) \Leftrightarrow (1/2^j) \log \delta_j^{-1} \to 0 \ (j \uparrow \infty).$$

(2) Let

$$\Omega(r) = \begin{cases} \exp(r/\log^\sigma r), & r \geqslant e^\sigma, \\ \Omega(e^\sigma), & 1 \leqslant r \leqslant e^\sigma, \end{cases} \quad \sigma > 1;$$

$$(8.2) \Leftrightarrow \delta_j^{-1}/j^\sigma \text{ is bounded};$$

$$(8.3) \Leftrightarrow \delta_j^{-1}/j^\sigma \to 0 \ (j \uparrow \infty).$$

In the first example (8.2) is stronger than (8.3) but in the second one the opposite occurs.

Notice that since $\Omega(r) \geqslant r^{d-1}$ (8.2) implies easily the finiteness of ψ.

APPENDIX B: MOSER–DEIFT–SIMON INEQUALITY ON KAM SPECTRA

Deift–Simon,[3] extending an idea of Moser,[30] showed that, for general, almost periodic potentials,

$$\lim_{\epsilon \downarrow 0} \frac{\alpha^2(E+\epsilon) - \alpha^2(E-\epsilon)}{2\epsilon} \geqslant 1, \quad E \text{ a.e. in } S. \qquad (B1)$$

Here we want to discuss briefly the constructive version of (B1) for $L^{(\epsilon)}$, namely, we sketch the proof of

$$\frac{d}{dE} \alpha^2 \geqslant 1, \quad E \in \tilde{\mathbf{E}}^{(\epsilon)}, \quad \frac{d}{dE} \equiv \text{Whitney derivative}. \qquad (B2)$$

Without loss of generality we can assume that $\hat{W}_0 = 0$ and, to simplify the Hamiltonian formalism, we consider $V \equiv 0$ in which case $H_{\epsilon W} = \sqrt{E} A_1 + \omega_2 A_2 + \cdots + \omega_d A_d - (\epsilon/\sqrt{E}) A_1 \sin^2 \theta_1 \, W(\theta_2,...,\theta_d)$. Then we have

$$\alpha(E) = \sqrt{E} + \epsilon \hat{F}_0^{(0)} + \epsilon^2 \hat{F}_0^{(1)} + O(\epsilon^4)$$

with $F^{(0)} \equiv -(\sin^2 \theta_1/\sqrt{E}) W(\theta_2,...,\theta_d)$ and $F^{(1)}$ as in the inductive Lemma 6.1. Here $\hat{W}_0 = 0$ implies $\hat{F}_0 = 0$. Now, setting $\tilde{\omega} \equiv (\omega_2,...,\omega_d)$, a computation shows that

$$\begin{aligned} \hat{F}_0^{(1)} &= \int \frac{\partial \Phi_0}{\partial \theta_1} F^{(0)} + O(\epsilon) \\ &\equiv \int \left(\sum_{0 < |\nu| < N_0} \frac{\hat{F}_\nu^{(0)}}{-i\omega^{(0)} \cdot \nu} \right) F^{(0)} + O(\epsilon) \\ &= \frac{1}{2} \sum_{\substack{\mu \in \mathbb{Z}^{d-1} \\ |\mu| < N_0}} \frac{|\hat{W}_\mu|^2}{(\mu \cdot \tilde{\omega})^2 - 4E} + O(\epsilon), \end{aligned}$$

so that

$$\frac{d\alpha^2}{dE} = 1 + \epsilon^2 \frac{\sqrt{E}}{2} \sum_{|\mu| < N_0} \frac{|\hat{W}_\mu|^2}{[(\mu \cdot \tilde{\omega})^2 - 4E]^2} + \frac{1}{\sqrt{E}} O(\epsilon^3).$$

The smallness of the parameter $\epsilon\tau$ confirms (B2).

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On the construction of perfect Morse functions on compact manifolds of coherent states

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Perfect Morse functions on the manifold of coherent states are effectively constructed. The case of a compact, connected, simply connected Lie group of symmetry, having the same rank as the stationary group of the manifold of coherent states, such that the manifold of coherent states is a Kählerian C-space, is considered. It is proved that the set of perfect Morse functions is dense in the set of energy functions for linear Hamiltonians in the elements of the Cartan algebra of the Lie algebra of the representation of the group considered. It is proved that the maximum number of orthogonal vectors on a coherent vector manifold is equal to the Euler–Poincaré characteristic of the manifold.

I. INTRODUCTION

Particular attention has been paid lately to the application of geometrical ideas and methods in physics. First, geometrical ideas, especially symplectic structures,[1] have an important role in classical mechanics.[2] Second, the geometry of classical phase space is the starting point of the geometrical quantization program.[3,4] On the other hand, the right application of the variational principles in quantum physics is conditioned on the establishment of the topological and global geometrical properties of quantum state manifolds.[5]

Global variational methods are studied by means of the Morse theory. It is often useful to find the absolute minima of given functionals. In solving this difficult problem, Morse inequalities[6–8] can be successfully used. Morse inequalities imply constraints on the stable and unstable critical manifolds, imposed by the topology of the spaces on which the variational problems are considered. Morse inequalities have been applied to classical mechanics,[9] the Hartree–Fock problem,[10,11] and in connection with supersymmetry theories.[12] The extended Morse inequalities have been used in connection with the symmetry breaking phenomena for a Lie group of symmetry for Higgs–Landau systems.[13] Atiyah and Bott have applied Morse theory to determine the manifold of minima for the Yang–Mills functional in the equivariant case for Riemannian surfaces and the gauge group $U(n)$.[7] Another trend of applications of Morse theory in mathematical physics is the use of the Lusternick–Schnirelman theory (see, e.g., Ref. 14).

Morse inequalities become equalities for perfect Morse functions. The number of critical points of a given index of a perfect Morse function is minimal and is a topological invariant (the Betti number) of the manifold on which the variational problem is based. In the quantum case, many quantum states (e.g., the coherent[15,16] state manifolds for Lie groups of symmetry) are obtained by embedding of some symplectic manifolds in Hilbert spaces of state vectors.[5,17] Generally, these manifolds have locally phase space structures, but do not admit global canonical coordinates.[1,2] However, the corresponding quantum dynamical problems are global analysis problems. The perfect Morse functions just provide an economical method for the effective description of the geometry of quantum state manifolds. These functions exist only on manifolds that have torsion-free cohomology groups.[18,19] They provide a cell decomposition of the manifold in Morse–Borel cells.[20]

Many authors have been interested in the construction of perfect Morse functions. The ideas go back to papers of Bott[18,19] (see also Ref. 21). Let G be a compact connected Lie group with Lie algebra $\mathfrak{g}$, $\mathfrak{t}$ a Cartan subalgebra of $\mathfrak{g}$, and $X \in \mathfrak{g}$ a regular element such that $\mathfrak{t}$ equals the centralizer of X. Then $f: O(Y) \to \mathbf{R}$, $f(Z) = \langle Z, X \rangle$ is a perfect Morse function and the number of critical points of f is equal to the Euler–Poincaré characteristic of $\mathfrak{t}$. Here $O(Y) = \mathrm{Ad}(G)Y$, $Y \in \mathfrak{g}$, and $\langle\ ,\ \rangle$ is an Ad-invariant product in $\mathfrak{g}$. In our case the coherent state manifold is a compact, simply connected homogeneous Kähler manifold (Kählerian C-space[22]) (cf. Refs. 1 and 23, see also Sec. III). The fact that these manifolds admit perfect Morse functions was proved by Bott[18,19] (see also references to papers of Borel). Frankel has extended the results of Bott to some classes of Kähler manifolds, not necessarily homogeneous.[24] Also Frankel gives examples of Morse functions for classical groups using the trace function[25] (see also Refs. 26 and 27). Takeuchi[28] has studied large classes of real and complex symmetric R-spaces (in the complex case these are the irreducible Hermitian symmetric spaces) that admit perfect ("economical"[29]) Morse functions, using (Nagano's) zonal spherical functions. Another idea is to embed the manifolds into suitable Euclidean spaces and apply Morse theory to the length function.[27,30] Flag manifolds[31–33] are embedded in the projective space by means of Plücker embedding and the perfect Morse function on projective space is used.[8]

In this paper, perfect Morse functions are constructed on coherent state manifolds admitting a Kählerian C-space structure. These functions have the significance of energy functions associated to the Hamiltonian.

Section II comprises elements of Morse theory on a manifold of quantum states: Morse inequalities and properties of perfect Morse functions.

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In Sec. III, perfect Morse functions are effectively constructed as energy functions associated with linear quantum systems, described by coherent state manifolds for Lie groups of symmetry. The cellular structure of these manifolds and the maximal orthonormal systems of coherent vectors are deduced.

Some applications to the Slater determinant manifold are outlined in Sec. IV. The last section is devoted to concluding remarks.

II. MORSE INEQUALITIES ON A MANIFOLD OF QUANTUM STATES

(1) The conventional model of quantum mechanics attaches to every physical system a complex Hilbert space $\mathscr{H}$. To every wave vector $\phi\in\mathscr{H}^*=\mathscr{H}\setminus\{0\}$ the state $\tilde{\phi}=\{e^{i\varphi}\|\phi\|^{-1}\phi|\varphi\in\mathbb{R}\}$ is associated. The complex projective space of states is denoted by $\tilde{\mathscr{H}}$.

Let $\xi:\mathscr{H}^*\to\tilde{\mathscr{H}}$ be the projection $\xi(\phi)=\tilde{\phi}$, $\phi\in\mathscr{H}^*$. The unit sphere in $\mathscr{H}$ is defined as $\mathscr{S}(\mathscr{H})=\{\phi|\phi\in\mathscr{H};\ \|\phi\|=1\}$.

Let Q be a C^∞-differentiable manifold and let $\eta: Q\to\mathscr{S}(\mathscr{H})$ be an injective and continuous mapping so that each function f^ψ: $Q\to\mathbb{C}$, $f^\psi(p)=\langle\psi,\eta(p)\rangle$, $p\in Q$, $\psi\in\mathscr{S}(\mathscr{H})$ is differentiable. Here $\langle\ ,\ \rangle$ is the symbol of the scalar product of $\mathscr{H}$. The manifold $M=\eta(Q)$ is called the *quantum vector manifold*. If the restriction of the projection ξ to M is injective, then $\tilde{M}=\xi(M)$ is called the *quantum state manifold*. The structure of the differentiable manifold is canonically carried from Q onto M and $\tilde{M}$.

Differentiable functions f: $M\to\mathbb{R}$ will be studied later. As a typical example, functions $f_A(\psi)=\langle\psi,A\psi\rangle$ will be considered in Sec. III, where $\psi\in M$ and A is a self-adjoint operator with M in the domain.

(2) The Morse inequalities used further will be now outlined.[6–8,34–36]

Let f: $M\to\mathbb{R}$ be a smooth function on a compact, C^∞ m-dimensional manifold M. Let $\mathscr{C}_\nu(f)$ be the set of critical points of f, that is, the set of points when $df=0$. The Hessian $H(f)$ of f becomes a well-defined quadric form on the restriction of the tangent bundle of M to $\mathscr{C}_\nu(f)$. The number of negative (resp. 0) eigenvalues of the Hessian matrix at a critical point p is called the index of p (resp. the degeneracy degree) and is denoted by $\lambda_p(f)$. The connected submanifold $N\subset\mathscr{C}_\nu(f)$ is called the *nondegenerate critical manifold* for f if the degeneracy degree of all $p\in N$ equals the dimension of N. The latter condition means that the restriction $H_N(f)$ of the Hessian to the normal bundle of N is nondegenerate.

A function f on M is called a *nondegenerate (Morse) function in the extended sense* if $\mathscr{C}_\nu(f)$ is a union of nondegenerate critical manifolds. If N is a nondegenerate critical manifold of M, one may choose a subbundle $\nu_N^-(f)$ on the tangent bundle to M restricted to N on which $H_N(f)$ is negative definite. The fiber dimension of $\nu_N^-(f)$, denoted by λ_N, is called the index of N, and we say that N is orientable along f if and only if $\nu_N^-(f)$ is orientable. In the orientable case the *extended Morse (counting)* series for the Morse function f is defined, relative to a coefficient field K, as

$$M_t(f,K)=\sum_{N\subset\mathscr{C}_\nu(f)} t^{\lambda_N}P_t(N,K), \tag{2.1}$$

whereas in the nonorientable case the field K is $\mathbb{Z}_2$. Here $P_t(N,K)$ is the Poincaré series for N relative to a coefficient field K,

$$P_t(N,K)=\sum_{i=0}^{\dim N} t^i b_i(N,K), \tag{2.2}$$

and $b_i(N,K)$ is the Betti number relative to a field K, i.e., $b_i(N,K)=\dim H^i(N,K)$, $H^i(N,K)$ being the ith cohomology group of N with coefficients in the field K.

For a nondegenerate (Morse) function f in the extended sense, the Morse inequalities can be written compactly,

$$M_t(f,K)-P_t(M,K)=(1+t)R(t), \tag{2.3}$$

where $R(t)$ is a polynomial with non-negative coefficients.

Note also that for a nondegenerate Morse function in the extended sense, Eq. (2.1) can be put in the form

$$M_t(f,K)=\sum_{j=0}^{m} t^j C_j(f,K), \tag{2.4}$$

$$C_j(f,K)=\sum_{N\subset\mathscr{C}_\nu(f)} b_{j-\lambda_N}(N,K). \tag{2.5}$$

The Morse inequalities (2.3) can be written

$$C_\lambda(f,K)\geqslant b_\lambda(M,K),\quad 0\leqslant\lambda\leqslant m, \tag{2.6a}$$

$$\sum_{i=0}^{\lambda}(-1)^{\lambda-i}C_i(f,K) \geqslant\sum_{i=0}^{\lambda}(-1)^{\lambda-i}b_i(M,K),\quad 0\leqslant\lambda\leqslant m, \tag{2.6b}$$

$$\sum_{i=0}^{m}(-1)^{m-i}C_i(f,K)=\sum_{i=0}^{m}(-1)^{m-i}b_i(M,K)=\chi(M,K), \tag{2.6c}$$

where $\chi(M,K)=P_{-1}(M,K)$ denotes the Euler–Poincaré characteristic of M.

The Morse function f in the extended sense is perfect[7] (or economical[29]) if in Eq. (2.3) $R(t)\equiv 0$. From Eqs. (2.6) it follows that if all odd coefficients $C_j(f,K)$ of $M_t(f,K)$ vanish, f is a perfect Morse function in the extended sense (Morse lacunary principle) and $C_j(f,K)=b_j(M,K)$.

When $\mathscr{C}_\nu(f)$ consists of points alone, Eq. (2.5) reduces to

$$C_j(f,K)=\operatorname{card}\{p\in\mathscr{C}_\nu(f)|\lambda_p(f)=j\},\quad 0\leqslant j\leqslant m. \tag{2.7}$$

Note also that the set of Morse functions on a compact manifold is an open set, dense in the set of differentiable functions on M (relative to the C^2 topology[37]).

The existence of perfect Morse funtions on a compact manifold has other topological consequences. For example, perfect Morse functions can exist only on manifolds that have a torsion-free cohomology group.[18,19]

The compact manifolds M appearing in this paper admit a Kählerian C-space structure (cf. Ref. 1, p. 168 and Ref. 23), so the field $K=\mathbb{R}$ can be used. However, because the manifolds here are Hodge, it will be sufficient to take $K=\mathbb{Z}$. The existence of perfect Morse functions on Kähler C-spaces

is known.[18,19] More precisely, the homogeneous manifold $G/C(T)$, where G is a compact, connected, semisimple Lie group and $C(T)$ the centralizer of a toral subgroup T of G, admits perfect Morse functions and also admits a homogeneous Kähler structure.[18–20,38] Here we shall present a concrete realization of a perfect Morse function in local coordinates, indicating also the globalization for a compact manifold of coherent states admitting a Kählerian C-space structure. Also these manifolds have complex analytic cellular decomposition in the sense of Morse–Borel,[20,28,39–41] and this cell decomposition is the one as the CW complexes, identical to the decomposition of certain classical groups like the Grassmann manifolds.[42]

III. PERFECT MORSE FUNCTIONS ON COMPACT MANIFOLDS OF COHERENT STATES

(1) Lately, the coherent states have been intensively studied.[15,16] Now we shall introduce in a convenient manner the strictly necessary elements used in this paper.

A quantum system with symmetry (in the sense of Wigner[43] and Bargmann[44]) is characterized by a continuous homomorphism $\tilde{\pi}$ of a topological group G into a group of transformations $\tilde{G}$ of the space $\tilde{\mathscr{H}}$ which leaves invariant the transition probabilities

$$(\tilde{\pi}(g)\tilde{\phi},\tilde{\pi}(g)\tilde{\psi}) = (\tilde{\phi},\tilde{\psi}), \quad g\in G, \quad \tilde{\phi},\tilde{\psi}\in\tilde{\mathscr{H}}, \tag{3.1}$$

where

$$(\tilde{\phi},\tilde{\psi}) = \|\phi\|^{-1}\|\psi\|^{-1}|\langle\phi,\psi\rangle|^2, \quad \phi,\psi\in\mathscr{H}^*.$$

Let $\tilde{\psi}_0\in\tilde{\mathscr{H}}$ be a fixed state. The $\tilde{G}$ orbit containing $\tilde{\psi}_0$,

$$\tilde{M} = \tilde{G}\tilde{\psi}_0 = \{\tilde{\pi}(g)\tilde{\psi}_0 | g\in G\}, \tag{3.2}$$

is called the *manifold of coherent states*, and every $\tilde{\phi}\in\tilde{M}$ is called a coherent state.

The closed group

$$K = \{h\,|h\in G;\ \tilde{\pi}(h)\tilde{\psi}_0 = \tilde{\psi}_0\} \tag{3.3}$$

is also considered. Then $\tilde{\pi}(K)$ is a stationary group of the state $\tilde{\psi}_0$ and there exists the bijection $\tilde{\xi}: G/K\to\tilde{M}$, defined by $\tilde{\xi}(g') = \tilde{\pi}(g)\tilde{\psi}_0$, where $g' = gK\in G/K$. Let the notation $\tilde{\psi}(g') = \tilde{\xi}(g')$. Evidently, $\tilde{\xi}(\theta') = \tilde{\psi}_0$, where θ is the unity element of the group G.

Further, G will be taken as a compact, connected Lie group. The fact that rank G = rank K will result in the next paragraph from general considerations, when restrictions on the fixed state $\tilde{\psi}_0$ and representation $\tilde{\pi}$ will be imposed. Also, further it will result that K is the centralizer of a toral subgroup of G and, moreover, is connected. The manifold $\tilde{M}$ will be endowed with the canonical differentiable (even real analytic) structure induced by $\tilde{\xi}$ from the homogeneous space G/K, hence $\tilde{M}$ is a quantum state manifold diffeomorphic with G/K. On the other hand, according to a theorem of Wigner and Bargmann,[43,44] there exists a continuous, unitary representation π of the group G onto the complex Hilbert space $\mathscr{H}$, such that

$$\widetilde{\pi(g)}\psi = \tilde{\pi}(g)\tilde{\psi}, \quad g\in G, \quad \psi\in\mathscr{H}^*. \tag{3.4}$$

Then, there exists the cross section σ: $\tilde{M}\to\mathscr{S}(\mathscr{H})$, where σ is an injective mapping such that $\xi(\sigma(\tilde{\psi}(g'))) = \tilde{\psi}(g')$, $g'\in G/K$. Let the notations $M = \sigma(\tilde{M})$, $\psi(g') = \sigma(\tilde{\psi}(g'))$, $\psi_0 = \sigma(\tilde{\psi}_0)$. It follows that M is a differentiable manifold relative to the structure induced by σ from $\tilde{M}$. The manifold M is named a *coherent vector manifold*, and every $\phi\in M$ is called a *coherent vector*. However, M is not a submanifold of $\mathscr{H}$.

Let us also introduce the mapings ξ_0: $M\to\tilde{M}$ and η: $G/K\to M$ by $\xi_0(\psi(g')) = \tilde{\psi}(g') = \tilde{\xi}(g')$, $g'\in G/K$, and $\eta(g') = \sigma\circ\tilde{\xi}(g') = \sigma(\tilde{\psi}(g')) = \psi(g')$. Evidently, ξ_0, η, and $\tilde{\xi} = \xi_0\circ\eta$ are diffeomorphisms. It follows that *the coherent state manifold $\tilde{M}$, the coherent vector manifold M, and the homogeneous space G/K are diffeomorphic.* It can be noted that M is a system of coherent vectors of type (π,ψ_0) in the sense of Perelomov[15] [local sections of the holomorphic line bundle $\xi^{-1}(\tilde{M})\to\tilde{M}$].

The previous construction is natural from the point of view of the interpretation of symmetries in quantum mechanics. Moreover, this construction is important for establishing the global properties of coherent state and coherent vector manifolds.

(2) Further, we need some elements of the theory of finite-dimensional representations of compact, connected, simply connected Lie groups (see, for example, Ref. 45). Because we deal with coset spaces G/K (rank K = rank G), there is no loss in generality in assuming that G is semisimple and simply connected (see, e.g., Ref. 46, p. 490).

Now, let T be a Cartan subgroup of the group G, and suppose that ψ_0 is a j-dominant weight vector relative to the representation π. Let $\mathscr{H}_j$ denote the complex linear covering of the manifold M. Let π_j denote the restriction of the representation π to $\mathscr{H}_j$. Hence π_j is a finite-dimensional unitary irreducible representation of the group G onto the complex linear space $\mathscr{H}_j$. There exists an isomorphism π_j' of the Lie algebra $\mathfrak{g}$ of the group G onto the Lie algebra $\pi_j'(\mathfrak{g})$ of the group $\pi_j(G)$ such that

$$\pi_j(e^X) = \exp(\pi_j'(X)), \quad X\in\mathfrak{g}, \tag{3.5}$$

where e: $\mathfrak{g}\to G$ and exp: $\pi_j'(\mathfrak{g})\to\pi_j(G)$ are exponential mappings.

Let us also fix a Cartan–Weyl base[47] of the complexification $\mathfrak{g}^c$ of the Lie algebra $\mathfrak{g}$, with elements h_i, e_α, $1\leqslant i\leqslant r$, $\alpha\in\Delta$, where r is the rank of the group G and Δ is a system of nonzero roots satisfying the commutation relations

$$[h_i,h_j] = 0, \quad [h_i,e_\alpha] = \alpha(h_i)e_\alpha, \tag{3.6a}$$

$$[e_\alpha,e_{-\alpha}] = \sum_{i=1}^{r}\alpha(h_i)h_i, \tag{3.6b}$$

$$[e_\alpha,e_\beta] = 0, \quad \alpha+\beta\notin\Delta\cup\{0\}, \tag{3.6c}$$

$$[e_\alpha,e_\beta] = N_{\alpha\beta}e_{\alpha+\beta}, \quad \alpha+\beta\in\Delta, \tag{3.6d}$$

where $1\leqslant i\leqslant j\leqslant r$, $\alpha,\beta\in\Delta$, and $\alpha(h_i)$, $N_{\alpha\beta}$ are real structure constants (cf. Ref. 47, pp. 166–171). If $\alpha+\beta\neq 0$, then the roots e_α, e_β are orthogonal relative to the Killing form $B(\cdot,\cdot)$, and the relation $\alpha(h) = B(h,h_\alpha)$, where $h_\alpha = [e_\alpha,e_{-\alpha}]$ was taken into account in Eq. (3.6b). The root system Δ is included in the dual $\mathfrak{t}^*$ of the Cartan algebra $\mathfrak{t}$ of T, and by means of the mapping $\alpha\to h_\alpha$, Δ can be embedded in $\mathfrak{t}$.

The elements h_i $(1\leqslant i\leqslant r)$ form a base of the complexification $\mathfrak{t}^c$ of the Cartan algebra $\mathfrak{t}$.

Let Π denote the set of simple roots. The simple roots can be chosen such that

$$\alpha_i(h_j)=\delta_{ij},\quad \alpha_i\in\Pi,\quad 1\leqslant i,\quad j\leqslant r. \tag{3.7}$$

Every root $\alpha\in\Delta$ is a linear combination of simple roots from Π with integer coefficients of the same sign. If these coefficients are non-negative, the root α is called a positive root. Let Δ_+ denote the set of positive roots.

Let $\mathscr{C}$ be the fundamental Weyl chamber

$$\mathscr{C}=\left\{w\middle| w=\sum_{i=1}^{r}\lambda_i w_i,\ \lambda_i\in\mathbb{Z}_+\right\}, \tag{3.8}$$

where the fundamental weights $w_i\in\mathfrak{t}^*$ verify the relations

$$2(w_i,\alpha_j)=\delta_{ij}(\alpha_j,\alpha_j),\quad 1\leqslant i,\quad j\leqslant n. \tag{3.9}$$

Here $(\cdot,\cdot)$ denotes the Euclidean scalar product in $\mathfrak{t}^*$.

The representations π_j and π_j' can be uniquely extended to the group homomorphism $\pi_j^*: G^c\to\pi_j(G^c)$ and, respectively, Lie algebra isomorphism $\pi_j^{*\prime}:\mathfrak{g}^c\to\pi_j^{*\prime}(\mathfrak{g}^c)$ by

$$\pi_j^*(e^Z)=\exp(\pi_j^{*\prime}(Z)),\quad Z\in\mathfrak{g}^c, \tag{3.5'}$$

where $\pi_j^{*\prime}(\mathfrak{g}^c)$ is the complexification of the Lie algebra $\pi_j'(\mathfrak{g})$, but G^c and $\pi_j^*(G^c)$ denote the complexification of the groups G and, respectively, $\pi_j(G)$. Of course, $\pi_j^*(G^c)$ and $\pi_j^{*\prime}(\mathfrak{g}^c)$ are the sets of linear operators on $\mathscr{H}_j$. Also let

$$H_i=\pi_j^{*\prime}(h_i),\quad E_\alpha=\pi_j^{*\prime}(e_\alpha), \tag{3.10}$$

where $1\leqslant i\leqslant n$ and $\alpha\in\Delta$. According to the theory of compact representations,[38] the j-dominant weight can be chosen to belong to the Weyl chamber $\mathscr{C}$ and

$$\begin{aligned} &H_i\psi_0=j_i\psi_0,\quad 1\leqslant i\leqslant r,\\ &E_{-\alpha}\psi_0\neq 0,\quad \alpha\in\Delta',\\ &E_{-\alpha}\psi_0=0,\quad \alpha\in\Delta\setminus\Delta', \end{aligned} \tag{3.11}$$

where $j=(j_1,\ldots,j_r), j_i=(\omega_i,j), i=1,\ldots,r$, and

$$\Delta'=\{\alpha|\alpha\in\Delta;\ (j,\alpha)<0\}. \tag{3.12}$$

The base of the real Lie algebra $\mathfrak{g}$ [resp. $\pi_j'(\mathfrak{g})$] is made of elements ih_k, $i(e_\alpha+e_{-\alpha})$, $e_\alpha-e_{-\alpha}$ [resp., the anti-Hermitian operators iH_k, $i(E_\alpha+E_{-\alpha})$, $E_\alpha-E_{-\alpha}$, $1\leqslant k\leqslant r$, $\alpha\in\Delta$].

Also, the unitarity of the representation π_j implies

$$H_i^{+}=H_i,\quad E_\alpha^{+}=E_{-\alpha},\quad 1\leqslant i\leqslant r,\quad \alpha\in\Delta, \tag{3.13}$$

where A^{+} denotes the adjoint of the operator A.

Let $\mathfrak{p}$ denote the complex Lie algebra with base $h_i, e_{-\alpha}$, $1\leqslant i\leqslant r$, $\alpha\in\Delta\setminus\Delta'$. The complex Lie subgroup $P=e^{\mathfrak{p}}$ of the group G^c is a parabolic group corresponding to the parabolic subset $-(\Delta\setminus\Delta')$ of Δ (cf. Ref. 45, p. 54) (Borel group if $\Delta'=-\Delta_+$). The representation $\tilde{\pi}_j$ is irreducible, $K=G\cap P$, and

$$P=\{g|g\in G^c;\ \widetilde{\pi_j(g)\psi_0}=\tilde{\psi}_0\}. \tag{3.14}$$

It follows that there is a diffeomorphism of homogeneous spaces c: $G/K\to G^c/P$, defined by $c(gK)=gP$, $g\in G$.[38] The following facts are known about the homogeneous space G^c/P strictly associated to the irreducible representation $\tilde{\pi}_j$ of dominant weight j.[1,20,22,38] The space G^c/P is algebraic. The isotropy group $K=G\cap P$ is connected, with the same rank as G and it is the centralizer of a torus in G (K is a maximal torus if P is a Borel subgroup). The principal bundle $P\to G^c\to G^c/P$ is holomorphic. Details on the geometric realization are provided by the Bott–Borel–Weil theorem (see, e.g., Ref. 45, p. 201). Following the denomination of Wang,[22] G^c/P is a C-space, endowed with a Kählerian structure.

Let $W(G)$ denote the Weyl group[47] associated with G, defined as the quotient $W(G)=N(T)/C(T)$ of the normalizer

$$N(T)=\{g|g\in G;\ gTg^{-1}=T\} \tag{3.15}$$

of the Cartan group T by the corresponding centralizer $C(T)=\{g|g\in G;\ gt=tg,\ \text{any } t\in T\}$. Similarly, $W(K)$ denotes the Weyl group associated with the group K. Let $\Sigma\subset N(T)$ be a set of elements such that the quotient space $W(G)/W(K)$ is made of the coset classes $(sC(T))W(K)$, $s\in\Sigma$. Let us define the mappings $\tilde{s}$: $\Delta\to\Delta$, for every $s\in\Sigma$, by

$$\tilde{s}_\alpha(h)=\alpha(s^{-1}hs),\quad h\in\mathfrak{t},\quad \alpha\in\Delta. \tag{3.16}$$

The action of $\tilde{s}_\alpha$ on an element k of the space generated by Δ is the reflection

$$\tilde{s}_\alpha(k)=k-2(\alpha,k)\alpha/(\alpha,\alpha), \tag{3.17}$$

and for every $\alpha\in\Delta$, there exists $\beta\in\Delta$ and $\gamma\in\Pi$ such that $\alpha=\tilde{s}_\beta(\gamma)$.

(3) With the previous facts, the Kählerian structure of the homogeneous space G^c/P will be carried onto the manifold M of coherent vectors. Moreover, the Kählerian structure of the homogeneous space G^c/P will be also transported onto the homogeneous space G/K.To get the Kählerian structure on G^c/P, here we use local coordinates. The effective construction of a Kähler metric on a compact manifold of coherent states in the case of nonsingular highest weight was pointed out in Ref. 23. The same argument as in Ref. 23 provides the globalization in the present construction.

Let us introduce the vectors

$$\Phi_z=\exp\left(\sum_{\alpha\in\Delta'}z_\alpha E_{-\alpha}\right)\psi_0, \tag{3.18}$$

$$\psi_z=\|\Phi_z\|^{-1}\Phi_z=\psi(g')\in M, \tag{3.19}$$

for

$$c(g')=\exp\left(\sum_{\alpha\in\Delta'}z_\alpha E_{-\alpha}\right)P, \tag{3.20}$$

where z belongs to the m-dimensional Euclidean complex space $\mathbb{C}^m$ and

$$2m=\dim\tilde{M}=\dim M=\dim G/K=\dim G^c/P. \tag{3.21}$$

Let the notation

$$\mathscr{V}_0=\{\psi_z|z\in\mathbb{C}^m\}$$

and let us consider the homeomorphism h: $\mathscr{V}_0\to\mathbb{C}^m$, defined by $h^{-1}(z)=\psi_z$. Let also the notation $\mathscr{V}_s=\pi_j(s)\mathscr{V}_0$ and $h_s=h\circ\pi_j(s)^{+}$ for every $s\in\Sigma$. Then $(\mathscr{V}_s)_{s\in\Sigma}$ *is an open, finite covering of the manifold M, and the collection of local charts $(\mathscr{V}_s, h_s)_{s\in\Sigma}$ generates an atlas of a Kählerian manifold with the fundamental two-form on $\mathscr{V}_0$*

$$\omega=-i\sum_{\alpha,\beta\Delta}g_{\alpha\bar{\beta}}\,dz_\alpha\wedge d\bar{z}_\beta,$$

where

$$g_{\alpha\bar{\beta}} = \frac{\partial^2 F(z,\bar{z})}{\partial z_\alpha \, \partial \bar{z}_\beta}, \tag{3.22}$$

$$F(z,\bar{z}) = \ln\langle \Phi_z, \Phi_z \rangle. \tag{3.23}$$

Note that ω is nonsingular everywhere.[23]

The Kählerian structure of the manifold M is induced by the mapping ξ_0 onto the coherent state manifold $\tilde{M}$.

To every linear operator A on $\mathscr{H}_j$, a function $f_A : \tilde{M} \to \mathbb{C}$ can be associated by

$$f_A(\tilde{\psi}) = \langle \psi, A\psi \rangle, \quad \psi \in M, \tag{3.24}$$

called the *covariant symbol*.[48] If A is a Hermitian operator associated to an observable, then f_A is a real function, and $f_A(\tilde{\psi})$ can be interpreted as an expectation value of the considered observable. If H is a Hamiltonian, then f_H is called an energy function. The manifold $\tilde{M}$ (being Kählerian) is, of course, also symplectic, hence the symbol f_A associated to a Hermitian operator admits the interpretation of a classical observable.

Let us now introduce the notation

$$\lambda_\alpha = \sum_{i=1}^{r} \epsilon_i \alpha(h_i), \quad \epsilon = (\epsilon_1, \ldots, \epsilon_r) \in \mathbb{R}^r. \tag{3.25}$$

After this long preparation, we are ready to state the main theorem of the paper.

Theorem 1: Let $\tilde{M}$ be the homogeneous compact manifold of coherent states, diffeomorphic with G/K and the Kählerian C-space G^c/P. Here G is a compact, connected, simply connected Lie group and K is a closed subgroup (connected and rank K = rank G). Then the energy function f_H associated to the Hamiltonian

$$H = \sum_{i=1}^{r} \epsilon_i H_i, \quad \epsilon = (\epsilon_1, \ldots, \epsilon_r) \in \mathbb{R}^r, \tag{3.26}$$

is a perfect Morse function in the extended sense. The nondegenerate critical manifolds of $\tilde{M}$ are described by $\tilde{\psi}^s_{z,c,r} = \widetilde{\pi_j(s)\psi_{z,c,r}}$, $s \in \Sigma$, where

$$\psi_{z,c,r} = \exp\left(\sum_{\alpha \in \Delta' \setminus \Delta''} z_\alpha E_{-\alpha} \right) \psi_0, \tag{3.27}$$

$$\Delta'' = \{\gamma \mid \gamma \in \Delta', \ \lambda_\gamma \neq 0\}. \tag{3.28}$$

Every nondegenerate critical manifold has even index

$$\lambda_{s,c,r} = 2 \operatorname{card}\{\alpha \mid \alpha \in \Delta'', \ \lambda_{\tilde{s}_\alpha} > 0\}, \quad s \in \Sigma. \tag{3.29}$$

Moreover, if

$$\lambda_{\tilde{s}_\alpha} = \sum_{i=1}^{r} \epsilon_i \tilde{s}_{\alpha_i}(h_i) \neq 0, \quad s \in \Sigma, \quad \alpha \in \Delta', \tag{3.30}$$

then the associated energy function f_H is a perfect Morse function.

Proof: Let us consider the function $f: \mathbb{C}^m \to \mathbb{R}$ defined by

$$f(z,\bar{z}) = \langle \psi_z, H\psi_z \rangle, \quad z \in \mathbb{C}^m. \tag{3.31}$$

The function f can be put into the form

$$f(z,\bar{z}) = \sum_{i=1}^{r} \epsilon_i j_i - \sum_{\gamma \in \Delta'} \lambda_\gamma z_\gamma \frac{\partial F(z,\bar{z})}{\partial z_\gamma}. \tag{3.32}$$

Indeed, from Eqs. (3.18) and (3.19) it follows that

$$f(z,\bar{z}) = \|\Phi_z\|^{-2} \langle \Phi_z, He^X \psi_0 \rangle, \tag{3.33}$$

where

$$X = \sum_{\alpha \in \Delta'} z_\alpha E_{-\alpha}. \tag{3.34}$$

But

$$He^X = e^X \sum_{n \geq 0} (n!)^{-1} (-\operatorname{ad} X)^n H, \tag{3.35}$$

where, taking into account Eqs. (3.26), (3.25), (3.34), (3.10), and (3.6a),

$$(\operatorname{ad} X) H = [X, H] = \sum_{\alpha \in \Delta'} z_\alpha \lambda_\alpha \frac{\partial X}{\partial z_\alpha}, \tag{3.36}$$

$$(\operatorname{ad} X)^n H = \sum_{\alpha \in \Delta'} z_\alpha \lambda_\alpha (\operatorname{ad} X)^{n-1} \frac{\partial X}{\partial z_\alpha}, \quad n \geq 2. \tag{3.37}$$

Equation (3.35) becomes

$$\begin{aligned} He^X &= e^X H - \sum_{\alpha \in \Delta'} z_\alpha \lambda_\alpha e^X \\ &\quad \times \sum_{n \geq 0} (-1)^n ((n+1)!)^{-1} (\operatorname{ad} X)^n \frac{\partial X}{\partial z_\alpha} \\ &= e^X H - \sum_{\alpha \in \Delta'} \lambda_\alpha z_\alpha \frac{\partial e^X}{\partial z_\alpha}. \end{aligned} \tag{3.38}$$

From Eqs. (3.11) and (3.26),

$$H\psi_0 = \sum_{i=1}^{r} \epsilon_i j_i \psi_0, \tag{3.39}$$

and also

$$He^X \psi_0 = e^X \sum_{i=1}^{r} \epsilon_i j_i \psi_0 - \sum_{\alpha \in \Delta'} z_\alpha \lambda_\alpha \frac{\partial \Phi_z}{\partial z_\alpha}. \tag{3.40}$$

Introducing the latter expression in Eq. (3.33) and taking into account Eq. (3.23), the relation (3.32) is proved. Note that if the subspaces generated by $E_{-\alpha}$, where $\alpha \in \Delta'$ and $\alpha \in \Delta \setminus \Delta'$ are Abelian, all terms with $n > 1$ in Eq. (3.35) are 0. This situation corresponds to Hermitian symmetric manifolds (cf. Ref. 49, p. 1191).

The point $z \in \mathbb{C}^m$ is a critical point of the function f if and only if

$$\frac{\partial f}{\partial \bar{z}_\beta} = -\sum_{\gamma \in \Delta'} \lambda_\gamma z_\gamma \frac{\partial^2 F}{\partial z_\gamma \, \partial \bar{z}_\beta} = 0, \quad \beta \in \Delta'. \tag{3.41}$$

Since the fundamental two-form ω is nondegenerate, the matrix $\Gamma = (g_{\gamma\bar{\beta}})_{\gamma,\beta \in \Delta'}$ is nonsingular. Then Eq. (3.41) is equivalent to the conditions

$$\lambda_\gamma z_\gamma = 0, \quad \gamma \in \Delta'. \tag{3.42}$$

The manifold of critical points of f is

$$\mathscr{C}_r(f) = \{z \mid z \in \mathbb{C}^m; \ z_\gamma = 0, \ \gamma \in \Delta''\}, \tag{3.43}$$

where Δ'' is given by Eq. (3.28).

If the point $z_0 \in \mathscr{C}_r(f)$, then (3.41) and (3.42) imply

$$\left(\frac{\partial^2 f}{\partial z_\alpha \, \partial z_\beta} \right)_{z_0} = \left(\frac{\partial^2 f}{\partial \bar{z}_\alpha \, \partial \bar{z}_\beta} \right)_{z_0} = 0, \quad \alpha, \beta \in \Delta', \tag{3.44}$$

$$(W_{z_0}(f))_{\alpha\beta} = \left(\frac{\partial^2 f}{\partial z_\alpha \, \partial \bar{z}_\beta} \right)_{z_0} = -\lambda_\alpha g_{\alpha\bar{\beta}} = -g_{\alpha\bar{\beta}} \lambda_\beta. \tag{3.45}$$

From Eq. (3.45) it results that the positive definite matrix Γ and the matrix $\Lambda = (\lambda_\alpha \delta_{\alpha\beta})_{\alpha,\beta \in \Delta'}$ are simultaneously diagonalizable. So, the Hessian matrix of the function f in z_0,

$$H_{z_0}(f) = 2U\begin{pmatrix} W & 0 \\ 0 & W^t \end{pmatrix} U^+,$$
$$U = 2^{-1/2}\begin{pmatrix} \mathbf{1}_m & \mathbf{1}_m \\ i\mathbf{1}_m & -i\mathbf{1}_m \end{pmatrix}, \tag{3.46}$$

admits λ_- (resp. λ_0) negative (resp. 0) eigenvalues, where

$$\lambda_- = 2\,\mathrm{card}\{\gamma|\gamma\in\Delta';\ \lambda_\gamma > 0\},$$
$$\lambda_0 = 2\,\mathrm{card}\{\gamma|\gamma\in\Delta';\ \lambda_\gamma = 0\}, \tag{3.47}$$

and $\mathbf{1}_n$ denotes the unit matrix of the group $\mathrm{GL}(n,\mathbb{C})$ and W^t denotes the transpose of matrix W. In Eq. (3.46) the Hessian is expressed in the real coordinates (x_α, y_α), where $z_\alpha = x_\alpha + iy_\alpha$,

$$(H(f))_{\alpha\beta} = \begin{pmatrix} \dfrac{\partial^2 f}{\partial x_\alpha\,\partial x_\beta} & \dfrac{\partial^2 f}{\partial x_\alpha\,\partial y_\beta} \\ \dfrac{\partial^2 f}{\partial y_\alpha\,\partial x_\beta} & \dfrac{\partial^2 f}{\partial y_\alpha\,\partial y_\beta} \end{pmatrix}, \quad \alpha,\beta\in\Delta'. \tag{3.48}$$

Equations (3.44)–(3.47) imply that the Hessian matrix (3.48) has the nonzero determinant $\det(H(f))_{\alpha,\beta\in\Delta'} \neq 0$, hence the manifold (3.43) is a nondegenerate critical manifold. A point (vector) of this manifold has the expression (3.27).

Now, choosing $f^s = f_H \circ \xi_0 \circ \pi_j(s) \circ h^{-1}$, $s\in\Sigma$, it follows that the nondegenerate critical manifolds of $\tilde{M}$ for f^s are described by $\tilde{\psi}^s_{z,c,r} = \widetilde{\pi_j(s)\psi_{z,c,r}}$. Every nondegenerate critical manifold has even index (3.29).

It follows that in Eq. (2.1) the fiber of the nondegenerate critical manifold has even dimension, and, moreover, the coefficients $C_i(f)$ (2.5) are all even, hence the lacunary principle of Morse in the extended sense is applicable.

The first part of Theorem 1 was proved.

If $\Delta' = \Delta''$, then $z_0 = 0$ is the only critical point of the function f. This point is a nondegenerate one and has an even index (3.47).

If the conditions (3.30) are fulfilled, then it results that the critical points of the function f_H are the distinct states $\tilde{\psi}^s$, $s\in\Sigma$, where $\psi^s = \pi_j(s)\psi_0$. Every critical state $\tilde{\psi}^s$ is nondegenerate and has an even index

$$\lambda_s = 2\,\mathrm{card}\{\alpha|\alpha\in\Delta';\ \lambda_{\tilde{s}_\alpha} > 0\}. \tag{3.49}$$

Now, the lacunary principle of Morse is applied and the Theorem is proved.

Remark 1: The set of perfect Morse functions is dense in the set of energy functions associated to Hamiltonians which are linear in H_i, $i = 1,\ldots,r$.

Remark 2: As in the formulation of Bott's theorem[21] presented in the Introduction, Theorem 1 is also true for Hamiltonians H such that iH belongs to the Lie algebra $\pi'_j(\mathfrak{g})$. Note also that the case $iH\in\pi'_j(\mathfrak{g})$ corresponds to coherent state preserving Hamiltonians for semisimple Lie groups.[41] We also remember that Frankel has proved the existence of perfect Morse functions for linear Hamitonians in the generators of the Lie algebra of a group of isometries of a compact connected Kähler manifold.[24] Here the Kählerian structure of the compact coherent manifold follows, as was already pointed out, from the fact the $\tilde{M}$ is the orbit of the j-dominant weight (see also Ref. 1, p. 168). The existence of perfect Morse functions on Kählerian C-spaces was proved by Bott.[18,19,21]

Remark 3: The perfect Morse function f_H is related to the spherical zonal function used by Takeuchi in the case of irreducible symmetric complex and real R-spaces.[28] The complex R-spaces in the paper[28] of Takeuchi are the C-spaces of Wang.[22] In the complex case, the function of Takeuchi is constructed only for Hermitian symmetric spaces, whereas the proof presented here is valid for Kählerian C-spaces. In fact, in the case of complex Grassmann manifold Takeuchi[29] claims that the economical spherical function reduces to the "nice" function (of Hattori), which is a particular case of the function constructed in Sec. IV [see Eq. (4.11)]. On the other hand, the proof presented here in the case of the compact coherent state manifold is more direct.

As an application to Theorem 1, a description follows of a maximal system of coherent vectors.

Theorem 2: If $\mathscr{T}\subset M$ is a maximal orthogonal system of coherent vectors, then there exists an element $g\in G$ such that

$$\mathscr{T} = \{\pi_j(g)\psi^s|s\in\Sigma\} \tag{3.50}$$

and the number of vectors in $\mathscr{T}$ is equal to the Euler–Poincaré characteristic $\chi(M)$.

Proof: The perfect Morse function f_H appearing in Theorem 1 induces a cellular structure onto the manifold of coherent states $\tilde{M}$. For every $s\in\Sigma$ there exists in the cell $\tilde{\mathscr{V}}_s = \xi_0(\mathscr{V}_s)$ one and only one critical state $\tilde{\psi}^s$ of the function f_H. Observing that $\{\tilde{\mathscr{V}}_s\}_{s\in\Sigma}$ is an open covering of the manifold $\tilde{M}$, that the group $\tilde{G}$ acts transitively on M, and that

$$\langle\psi^s,\psi^{s'}\rangle = \delta_{ss'}, \langle\psi_0,\psi_z\rangle \neq 0, \tag{3.51}$$

for $s,s'\in\Sigma$, $z\in\mathbb{C}^m$, Eq. (3.50) follows. On the other hand, from the Morse equality (2.6c) with all odd Betti numbers equal to 0, it can be deduced that Σ and $\mathscr{T}$ have exactly $\chi(M)$ elements.

IV. APPLICATIONS TO THE MANIFOLD OF SLATER DETERMINANTS

From the preceding section, it can be noted that the results outlined there are applicable to large classes of quantum systems with symmetry, where G is compact and rank-G = rank K, and admit a Kählerian C-space structure. The situation when the manifold $\tilde{M}$ is endowed with a homogeneous complex structure includes the Hermitian symmetric spaces [in fact, this situation occurs when dim(center K) = 1, and there are only two invariant structures (see, e.g., Ref. 46, p. 505). This situation also corresponds exactly to the case when the subspaces generated by $E_{-\alpha}$, where $\alpha\in\Delta'$ and $\alpha\in\Delta\setminus\Delta'$, both can be chosen as Abelian subalgebras of $\pi_j^{*\prime}(\mathfrak{g}^c)$.[49]

The irreducible Hermitian symmetric spaces (see Ref. 47, p. 518) appear frequently in different branches of physics. For example, $\mathrm{SU}(p+q)/S(\mathrm{U}(p)\times\mathrm{U}(q))$ appears in connection with Hartree–Fock problems[10] or Grassmann nonlinear σ models,[50] $\mathrm{SO}(2n)/\mathrm{U}(n)$ is present in fermion models[16] or in quantum field theoretical models as the Gross–Neveu type model,[48] $\mathrm{SO}(p+2)/\mathrm{SO}(p)\times\mathrm{SO}(2)$ is used in models with spins with $\mathrm{SO}(p)$ symmetry,[51] and $\mathrm{Sp}(n)/\mathrm{U}(n)$ is the manifold of Lagrangian subspaces of the

phase space.[52] Also, Fordy and Kulish have studied the generalization of nonlinear Schrödinger equation by getting the field components to take values in irreducible Hermitian symmetric spaces.[53] Here we sketch a short application of the general Theorem 1 to the Hartree–Fock case. Details will be presented elsewhere.

The time-dependent variational principle of Hartree–Fock is based on the Slater determinant manifold.[54] A geometrical description of this manifold will be achieved by means of perfect Morse functions and topological constraints onto the energy function will also be established.

Let us consider a fermion Fock space $\mathscr{H}$ with vacuum state $\tilde{\Omega}$. Let $\mathscr{H}_j$ denote the linear complex subspace of $\mathscr{H}$ with a base formed by the n-particle vectors

$$a_{p_1}^+ a_{p_2}^+ \cdots a_{p_n}^+ \Omega, \quad 1 \leqslant p_1 < p_2 \cdots < p_n \leqslant n', \tag{4.1}$$

where a_p^+, a_p $(p = 1,...,n')$ are the usual fermion creation and annihilation operators, respectively.

The Hartree–Fock Hamiltonian is a Hermitian operator on $\mathscr{H}_j$, realized as a second degree polynomial in bifermion operators

$$C_{pq} = a_p^+ a_q, \quad 1 \leqslant p, \leqslant n'. \tag{4.2}$$

From the usual anticommutation relations of the annihilation and creation operators, it follows that

$$[C_{pq}, C_{p'q'}] = \delta_{qp'} C_{pq'} - \delta_{pq'} C_{p'q}, \quad 1 \leqslant p, q \leqslant n'. \tag{4.3}$$

The Lie algebra of anti-Hermitian operators on $\mathscr{H}_j$, which are linear combinations with complex coefficients $x_{pq}, x_{pq} = -\bar{x}_{qp}$, of the operators C_{pq}, is isomorphic with the Lie algebra $u(n')$ of the group $\mathrm{U}(n')$. But the group $\mathrm{U}(n')$ is canonically isomorphic with the product of groups $\mathrm{U}(1) \times \mathrm{SU}(n')$, being, of course, connected, simply connected. Hence it can be chosen that $G = \mathrm{SU}(n')$. Let us also fix the initial vector

$$\psi_0 = a_1^+ a_2^+ \cdots a_n^+ \Omega. \tag{4.4}$$

Since

$$\begin{aligned} &C_{pq}\psi_0 = \delta_{pq}\psi_0, \quad 1 \leqslant p,q \leqslant n, \\ &C_{pq}\psi_0 = 0, \quad 1 \leqslant p \leqslant n', \quad n+1 \leqslant q \leqslant n', \\ &C_{pq}\psi_0 \neq 0, \quad n+1 \leqslant p \leqslant n', \quad 1 \leqslant q \leqslant n, \end{aligned} \tag{4.5}$$

ψ_0 is a vector of dominant weight $j = (1^n 0^{n'-n})$ of the unitary irreducible representation π_j of $\mathrm{SU}(n')$ on $\mathscr{H}_j$.

A manifold of coherent states of dimension $m = 2n(n'-n)$ is obtained,

$$\tilde{M} = \{\tilde{\psi} | \tilde{\psi} = \widetilde{\pi_j(g)\psi_0};\ g \in \mathrm{SU}(n')\}, \tag{4.6}$$

and is diffeomorphic with the complex Grassmann manifold $G_n(\mathbb{C}^{n'}) \approx \mathrm{U}(n')/\mathrm{U}(n) \times \mathrm{U}(n'-n)$.[11,55] The manifold of coherent vectors M is diffeomorphic with $\tilde{M}$, as in Sec. III. Here we introduce the notation

$$\begin{aligned} &\Phi_z = \exp\left(\sum_{p=n+1}^{n'} \sum_{q=1}^{n} \bar{z}_{qp} C_{pq}\right) \psi_0, \\ &\Sigma = \{\Delta^\sigma | \sigma \in S(n,n')\}, \\ &\Delta^\sigma = (\delta_{i\sigma(j)})_{1 \leqslant i,\ j \leqslant n'}, \end{aligned} \tag{4.7}$$

where $z = (z_{pq})_{\substack{n+1 \leqslant p \leqslant n' \\ 1 \leqslant q \leqslant n}} \in \mathbb{C}^{n(n'-n)}$ and the set $S(n,n')$ of $C_{n'}^{n'}$ Schubert symbols comprises all permutations σ: $\{1,2,...,n'\} \to \{1,2,...,n'\}$ with the property that its restrictions to the subsets $\{1,2,...,n\}$ and $\{n+1,...,n'\}$ are increasing. The atlas of the manifold M is generated by the open covering $\{\mathscr{V}_\sigma\}_{\sigma \in S(n,n')}$, where

$$\mathscr{V}_\sigma = \{\pi_j(\Delta^\sigma)\psi_z | z \in \mathbb{C}^{n(n'-n)}\}. \tag{4.8}$$

Here the local coordinate mappings h_σ: $\mathscr{V}_\sigma \to \mathbb{C}^{n(n'-n)}$ are

$$h_\sigma(\psi_{z\sigma}) = z, \quad \pi_j(\Delta^\sigma)^+ \psi_{z\sigma} = \psi_z, \quad \sigma \in S(n,n'). \tag{4.9}$$

The manifold M is called the *Slater determinant manifold* (in the second quantization).

According to Theorem 1, *the energy function f_{H_0} associated with the Hamiltonian*

$$H_0 = \sum_{i=1}^{n} c_i C_{ii}, \quad c_1 < c_2 < \cdots < c_n, \tag{4.10}$$

is a perfect Morse function.

By direct calculation[11] it is obtained, for $f = f_{H_0} \circ \xi_0 \circ \pi_j(\Delta^\sigma) \circ h_\sigma^{-1}$,

$$\begin{aligned} &f(z) = \mathrm{Tr}[(U + zVz^+)(\mathbf{1}_n + zz^+)^{-1}], \\ &U = (c_p \delta_{pq})_{1 \leqslant p,\ q \leqslant n}, \\ &V = (c_p \delta_{pq})_{n+1 \leqslant p,\ q \leqslant n'}. \end{aligned} \tag{4.11}$$

Then, the function f: $\mathbb{C}^{n(n'-n)} \to \mathbb{R}$ has a unique critical point $z = 0$. This point is nondegenerate, and the Hessian matrix has double degenerate eigenvalues: $c_q - c_p$, $1 \leqslant p \leqslant n < q \leqslant n'$.

The critical sets of the energy function f_{H_0} consists of the critical states $\tilde{\psi}_\sigma (\sigma \in S(n,n'))$, where

$$\psi_\sigma = a_{\sigma(1)}^+ a_{\sigma(2)}^+ \cdots a_{\sigma(n')}^+ \Omega, \tag{4.12}$$

and the critical state $\tilde{\psi}_\sigma$ has the index

$$\lambda_\sigma = 2\,\mathrm{card}\{(p,q) | 1 \leqslant p \leqslant n < q \leqslant n';\ \sigma(p) > \sigma(q)\}. \tag{4.13}$$

It is funny to recover directly the Betti numbers of the manifold M of Slater determinants[55]

$$\begin{aligned} &b_{2\lambda+1} = 0, \quad 0 \leqslant \lambda \leqslant n(n'-n), \\ &b_{2\lambda} = \mathrm{card}\{(\omega_1,...,\omega_n \in \mathbb{Z}_+^n | 0 \leqslant \omega_1 \leqslant \cdots \leqslant \omega_n \leqslant n'-n; \\ &\qquad \omega_1 + \omega_2 + \cdots + \omega_n = \lambda\}, \end{aligned} \tag{4.14}$$

and also the Euler–Poincaré characteristic $\chi(M) = C_n^{n'}$.

Remark 4: Observing that the uniparticle states are eigenstates with eigenvalues c_i, $i = 1,...,n$, it can be noted that perfect Morse functions are obtained when the uniparticle space is nondegenerate.

Remark 5: If the Hartree–Fock energy function f_H admits only nondegenerate critical states, then the Morse inequalities (2.6) are satisfied, where $0 \leqslant \lambda \leqslant m = 2n(n'-n)$, $C_\lambda(f)$ is the number of critical states of index λ for f_H, and the Betti numbers are given by (4.14). The problem of existence of Hartree–Fock states for Hamiltonians that do not have spurious states was analyzed in Ref. 10. The Hamiltonians that give the minimum number of Hartree–Fock states were effectively constructed here. It can also be shown that if the eigenvalues of the uniparticle states c_i are not all distinct, then the set of critical states are Grassmann submanifolds of the Grassmann manifold.

Remark 6: Perfect Morse functions of the type (4.11)

have been constructed in the mathematical literature for the Grassmann manifold (see, e.g., Refs. 31–33, where in the last reference, a calculation with components of matrices is performed). Note that the proof from Ref. 11 is more direct than the proofs of Refs. 32 and 33. Also in the case of Grassmann manifolds there are direct proofs that the Morse–Borel cells are identical to the Schubert cells.[40]

V. CONCLUSION AND DISCUSSION

The Morse inequalities in the classical and extended sense have been used for the effective construction of perfect Morse functions on a manifold of quantum states and quantum vectors. Actually, the case of a compact Lie group and of a compact manifold of coherent states having the structure of a Kählerian C-space was considered. It was proved that the set of perfect Morse functions is dense in the set of energy functions for linear Hamiltonians in the elements of the Cartan algebra of the Lie algebra of the representation of the considered group, which was chosen compact, connected, simply connected, and having the same rank as the stationary group of the manifold of coherent states. By the construction of perfect Morse functions, the cellular decomposition of the manifold of coherent states was found. For every energy function, the Morse inequalities are satisfied, the odd Betti numbers being in this case 0. Particularly, the energy function admits a number of critical points at least equal to the Euler–Poincaré characteristic of the manifold of coherent states. It is also proved that the Euler–Poincaré characteristic is equal to the maximum number of orthogonal vectors. The existence of perfect Morse functions for Kähler C-spaces is well established.[18,19,21] Here we have presented a construction of a perfect Morse function with physical significance as an energy function on the manifold of compact coherent states, diffeomorphic with Kählerian C-spaces.

The results obtained permit a correct approach to different problems of the classical limit and variational principles on manifold of coherent states from the point of view of global analysis and geometry. In this context, the cellular decomposition of the coherent state manifold induced by the perfect Morse functions is useful for solving asymptotical problems of actual interest such as the following: the classical limit of quantum collective models,[56,57] $1/N$ expansions in quantum field theory,[48] semiclassical behavior of functional integral based on coherent states,[58] Lagrangian analysis,[59] and the connection between the geometric quantization method and the functional integral.[52]

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Exponential time-evolution operator for the time-dependent harmonic oscillator

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The time-evolution operator for the time-dependent harmonic oscillator $H = \frac{1}{2}\{\alpha(t)p^2 + \beta(t)q^2\}$ is exactly obtained as the exponential of an anti-Hermitian operator. The method is based on the equations of motion for the coordinate and momentum operators in the Heisenberg representation. The problem is reduced to solving the classical equations of motion.

I. INTRODUCTION

The time-dependent Schrödinger equation (units are used so that $\hbar = 1$),

$$i\frac{\partial}{\partial t}U = HU, \quad U(t=0) = 1, \tag{1}$$

can be exactly solved for a number of simple problems. The solution is most conveniently written as a product of unitary operators.[1,2] However, in some cases it is preferable to look for a solution of the form

$$U = e^{-iA}, \tag{2}$$

where A is a Hermitian operator. When no exact solution is available exponential perturbation theories may be used. One of them is the celebrated Magnus expansion[3] that enables one to write A as $A_1 + A_2 + A_3 + \cdots$. The convergence of this series was extensively discussed.[4–6]

The applicability of the Magnus expansion to spin systems in periodic magnetic fields was investigated by Fel'dman[5] and Salzman.[6] To this end exactly solvable problems prove to be very useful.[5]

II. THE TIME-DEPENDENT HARMONIC OSCILLATOR

The purpose of this paper is to obtain the exponential time-evolution operator for the time-dependent harmonic oscillator

$$H = \tfrac{1}{2}\{\alpha(t)p^2 + \beta(t)q^2\}, \tag{3}$$

where α and β are real functions of t and $[q,p] = i$. Since the operators

$$H_1 = \tfrac{1}{2}q^2, \quad H_2 = \tfrac{1}{2}(qp + pq), \quad H_3 = \tfrac{1}{2}p^2, \tag{4}$$

span a three-dimensional Lie algebra there is a solution of (1) of the form (2) with[1]

$$A = b_1(t)H_1 + b_2(t)H_2 + b_3(t)H_3, \tag{5}$$

where $b_j, j = 1,2,3$ are real functions of t and $b_j(0) = 0$. It remains to determine the form of the b's.

The coordinate and momentum operators in the Heisenberg representation $q_t = U^+qU$ and $p_t = U^+pU$, respectively, satisfy

$$\frac{d}{dt}p_t = -\beta q_t, \quad \frac{d}{dt}q_t = \alpha p_t. \tag{6}$$

Therefore they can be written

$$p_t = P_p p + P_q q, \quad q_t = Q_p p + Q_q q, \tag{7}$$

where the P's and Q's obey the classical equations of motion

$$\frac{d}{dt}P_u = -\beta Q_u, \quad \frac{d}{dt}Q_u = \alpha P_u, \quad u = p,q, \tag{8}$$

with the boundary conditions $P_p(0) = Q_q(0) = 1$ and $P_q(0) = Q_p(0) = 0$. Only three of the four P's and Q's are independent since $[q_t,p_t] = i$ which leads to $P_pQ_q - P_qQ_p = 1$.

On using the well-known Baker–Campbell–Hausdorff formulas it is not difficult to prove that

$$\begin{aligned} &P_p = \cos\omega - b_2\omega^{-1}\sin\omega, \quad P_q = -b_1\omega^{-1}\sin\omega, \\ &Q_p = b_3\omega^{-1}\sin\omega, \quad Q_q = \cos\omega + b_2\omega^{-1}\sin\omega, \end{aligned} \tag{9}$$

where $\omega^2 = b_1b_3 - b_2^2$. When $\omega^2 < 0$ it is convenient to write $\omega = i\xi$, $\omega^{-1}\sin\omega = \xi^{-1}\sinh\xi$, and $\cos\omega = \cosh\xi$. Clearly, the form of the b's is completely determined by Eqs. (8) and (9) and the problem of finding U is solved.

Pechukas and Light[2] showed that U can also be written $U = \exp(ia_1H_1)\exp(ia_2H_2)\exp(ia_3H_3)$, where $a_1 = P_q/Q_q$, $a_2 = -\frac{1}{2}\ln Q_q$, and $a_3 = -Q_p/2Q_q$. Therefore the results of this paper also reveal the quite complex relationship between the two forms of writing U.

Apparently, the exponential time-evolution operator for the model just discussed was not obtained before. The method proposed here can be applied to other problems where the Hamiltonian operator can be written as a linear combination of the operators in a Lie algebra. Although the resulting expressions for U appear to be difficult to disentangle, they may be useful, for instance, in checking the applicability of the Magnus expansion.[2,3]

Spin systems in periodic magnetic fields[5,6] can be treated exactly in the same way if it is taken into account that

$$\begin{aligned} &M_x = \tfrac{1}{2}(q^2 + p^2), \quad M_y = \tfrac{1}{2}i(q^2 - p^2), \\ &M_z = -\tfrac{1}{2}i(qp + pq), \end{aligned} \tag{10}$$

and the Pauli spin matrices σ_x, σ_y, and σ_z obey the same commutation rules.

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Quadratic zeros of Racah 6j coefficients: A geometrical approach

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It is shown that the projective symmetries of the polynomial Φ of quadratic 6j coefficients form the symmetrical group S_6. Nonlinear rational symmetries of Φ are found. Partial parametrizations of the zeros of Φ are presented.

I. INTRODUCTION

Recently some progress has been made in finding zeros of 6j coefficients for the quadratic case.[1,2] Unlike the linear case[3,4] all solutions are not known.

In this paper we study the quadratic case from the point of view of geometry. All concepts of algebraic geometry used in this paper (projective coordinates, multiple points, base points, etc.) can be found in Semple and Roth.[5] Beyer, Louck, and Stein[6] have recently found that the polynomial of 6j coefficients is invariant under a symmetrical group S_6. In Sec. II, by studying some geometrical properties of the surface associated to the polynomial we also arrive at this symmetry group and show moreover that there is no other projective symmetry of the polynomial in the quadratic case. In Sec. III, we present rational nonlinear symmetries of the polynomial that we conjecture to generate an infinite group. In Sec. IV, two-dimensional cubic surfaces of zeros are found from geometrical considerations. These cubic surfaces, like those introduced by Bremner[7] for the linear case, can be rationally parametrized. However these parametrizations do not provide a complete parametrization of the four-dimensional surface of all zeros. By considering a family of cubic surfaces we arrive at a parametrization of a three-dimensional subvariety of zeros.

We take a *quadratic 6j coefficient* in the form

$$\begin{Bmatrix} (T+A+C-2)/2 & (S+A+B-2)/2 & (S+T+B+C-4)/2 \\ (T+B)/2 & (S+C)/2 & (S+T+A-2)/2 \end{Bmatrix},$$

where A, B, C, S, and T are integers $\geqslant 2$.

This 6j coefficient has exactly three decompositions in terms of extremal elements[4]:

$$(2-k)e_1+(S-k)e_2+(T-k)e_3+(A-2+k)e_4 + (B-2+k)e_5+(C-2+k)e_6+ke_7,$$

with $k=0$, 1, or 2 in the notations of Ref. 4.

The polynomial part of this 6j is given by

$$\Phi(A,B,C,S,T) = A(A-1)B(B-1)C(C-1) + 2ABCSTU + S(S-1)T(T-1)U(U-1), \quad (1)$$

where

$$U=2-A-B-C-S-T.$$

Using the notation $A^{(k)}=A(A-1)\cdots(A-k+1)$ and considering it as a symbolic exponential we can write Eq. (1) as

$$\Phi=(ABC+STU)^{(2)}.$$

II. SOME GEOMETRIC PROPERTIES OF THE SURFACE $\Phi=0$

We consider A, B, C, S, and T as belonging to $\mathbb{C}$, the field of complex numbers, and view the solutions of $\Phi=0$ as an algebraic surface (which we also call Φ) of complex dimension 4 in the projective space $P^5(\mathbb{C})$. More precisely, we introduce the homogenizing coordinate z, and the homogenization of Φ, which is of degree 6:

$$\Phi_H(A,B,C,S,T,z)=\Phi(A/z,B/z,C/z,S/z,T/z)z^6.$$

The projective coordinates A,B,C,S,T,z of a point of $P^5(\mathbb{C})$ are defined apart from a multiplicative factor. Points at infinity are those for which $z=0$.

Let us first study the multiple points of the surface Φ. To determine if a point M of the surface Φ is a multiple point we proceed in the following way. We take any other point $Q(\neq M)$ in $P^5(\mathbb{C})$ and parametrize the points of line MQ as

$$R(t)=Mt+Q(1-t) \quad (t\in\mathbb{C}).$$

The equation of degree 6 in t

$$\varphi_{M,Q}(t)=\Phi_H(R(t))=0,$$

for M and Q fixed, gives the intersection of line MQ with the surface Φ. The point M is multiple of multiplicity k if $t=0$ is a root of multiplicity k of $\varphi_{M,Q}(t)=0$ for any point Q.

The only multiple points of the surface Φ are triple and double points. There are 31 triple points, ten of which are at infinity (Table I, where the coordinates will be defined a little below). We use a notation for the triple points that makes easy the description of the system L of lines joining these points (Table II). The double points of Φ form a set of 195 lines that is also the set of lines of types c and d of system L. We can classify the triple points of Φ accordingly to the type of lines of system L going through them. The triple points fall in three classes (Table III) that also correspond to the difference of notations of the triple points.

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TABLE I. The 31 triple points. The indices k, l, m, i take the values 1, 2, ..., 6. Note that there are two notations for the 15 points like $T_{12} = T_{21}$ and 12 notations for the ten points at infinity like $T_{123} = T_{456} = T_{321} = \cdots$.

Number of points	Notation	Coordinates
6	T_k	$x_i = \delta_{ik},\ z = 1$
15	T_{kl} $k \neq l$	$x_i = \frac{1}{2} - \delta_{ik} - \delta_{il},\ z = 1$
10	T_{klm} $k \neq l \neq m \neq k$	$x_i = \frac{1}{2} - \delta_{ik} - \delta_{il} - \delta_{im},\ z = 0$

The six triple points $(T_k)_{1<k<6}$ are independent and form one of these classes. It is then very natural to introduce new projective coordinates $(x_i)_{1<i<6}$ such that the triple point T_k has coordinates $x_i = \delta_{i,k}$. The transformation from projective coordinates A, B, C, S, T, U (we use coordinate $U = 2z - A - B - C - S - T$ instead of z to make the transformation simpler) is given by

$$\begin{pmatrix} A \\ B \\ C \\ S \\ T \\ U \end{pmatrix} = \begin{pmatrix} 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{pmatrix}. \tag{2}$$

The transformation matrix in (2) has been chosen so that its column k represents the A, B, C, S, T, U coordinates of the triple point T_k with the determination corresponding to $z = 1$.

We recall that here, the projective coordinates A, B, C, S, T, U, or $(x_i)_{1<i<6}$ of a given point of $P^5(\mathbb{C})$ are defined apart from a multiplicative factor. Thus if we want that A, B, C, S, T, U correspond to our earlier definition of Eq. (1) we have to fix this multiplicative factor by $z = 1$. Since $z = \Sigma_{i=1}^{6} x_i$, this condition corresponds to the relation

$$\sigma_1 = \sum_{i=1}^{6} x_i = 1 \tag{3}$$

on the new coordinates.

TABLE II. System L of lines. Classification of the lines joining the triple points.

Type of lines	Number of lines	Lines	
a	30	$T_k T_{kl}$	meet Φ only at T_k and T_{kl}
b	120	$T_k T_l$	lines of simple points of Φ
		$T_{kl} T_{pq}$	
c	60	$T_k T_{lm} T_{klm}$	lines of double points of Φ passing through three triple points
d	135	$T_{klm} T_{pq}$ $(\neq T_{klm} T_{kl})$	lines of double points of Φ passing through two triple points
		$T_{klm} T_{pqr}$	

TABLE III. Classification of triple points. The three types of points, A, B, and C are characterized by different values of the numbers n_α, n_b, n_c, n_d of lines of types a, b, c, d of the system L through one triple point ($n_a + n_b + 2n_c + n_d = 30$).

Type of points	Number of points	Points	n_a	n_b	n_c	n_d
A	6	T_k	5	5	10	0
B	15	T_{kl}	2	14	4	6
C	10	T_{klm}	0	0	6	18

Transforming polynomial Φ_H by Eq. (2) gives, after dehomogenizing by $\sigma_1 = 1$ [Eq. (3)],

$$\Phi = \tfrac{1}{9}(\sigma_3 + \tfrac{1}{2})^2 - \tfrac{1}{5}(\sigma_5 + \tfrac{1}{4}), \tag{4}$$

where

$$\sigma_k = \sum_{i=1}^{6} x_i^k.$$

In this form it is clear that the polynomial Φ is invariant under any permutations of the x_i.

This symmetric group S_6 has also been found by Beyer, Louck, and Stein[6] in a more general setting (for $6j$ coefficients of any degree). However, with our approach we can now show in addition that there is no other projective symmetry of Φ. We intend by *projective symmetry* a projective transformation [in other words, this is a linear transformation of the $(x_i)_{1<i<6}$ coordinates] that leaves the surface Φ unchanged.

The system L of lines together with their types (a–d) and the triple points together with their classification are, of course, invariant under any projective symmetry ϑ of Φ. By considering the triple points of class A of Table III, we see that ϑ permutes the six triple points T_k,

$$\vartheta(T_k) = T_{\sigma(k)},$$

where σ is a permutation of 1,...,6.

Then by considering the lines of types a and c we have $\vartheta(T_{kl}) = T_{\sigma(k)\sigma(l)}$ and $\vartheta(T_{klm}) = T_{\sigma(k)\sigma(l)\sigma(m)}$. Since T_1, T_2, ..., T_6, and T_{12} form a basis of the projective space $P^5(\mathbb{C})$, the transformation ϑ is entirely determined by $\vartheta(T_1)$, ..., $\vartheta(T_6)$ and $\vartheta(T_{12})$, and so by the permutation σ. This shows that there is no other projective symmetry than the permutations of the x_k.

We now mention another remarkable property of the surface Φ which will be useful in Sec. IV. The 45 projective three-spaces $E_{(kl)(mn)}$ (where k, l, m, n are different integers $\leqslant 6$), defined by

$$x_k + x_l = 0, \quad x_m + x_n = 0,$$

are on the surface Φ. Moreover, there is no other projective three-space on Φ. Each of these spaces contains ten triple points, for example, $E_{(12)(34)}$ contains the points T_5, T_6, T_{13}, T_{14}, T_{23}, T_{24}, T_{135}, T_{136}, T_{145}, and T_{146}.

Let us point out that 27 of these spaces can be obtained at once from Eq. (1). For example, each term of Eq. (1) is zero if we set $A = S = 0$ (giving $E_{(23)(56)}$) or if we set

$A = S - 1 = 0$ (giving $E_{(23)(14)}$ since $1 - A - S = x_1 + x_4$ for dehomogenized x_i).

III. THE RATIONAL SYMMETRY Δ OF Φ

Equation (1) is invariant under two transformations R of coordinates A, B, C, S, T of the form

$$R(A,B,C,S,T) = (S,T,C + w,A,B).$$

Indeed forming $D = \Phi(A,B,C,S,T) - \Phi(S,T,C + w,A,B)$ we obtain a polynomial in w of degree 2:

$$D = a(w - w_1)(w - w_2).$$

But one root of D, w_1, corresponds to the permutation $A \leftrightarrow S$, $B \leftrightarrow T$, $C \leftrightarrow U$, which is an obvious rational symmetry of Eq. (1). It results that the symmetry corresponding to the other root of D, w_2, is also rational. More precisely we have

$$w_1 = 2 - A - B - S - T - 2C$$

and

$$w_2 = (1 - A - B - S - T) \times [(A^{(2)}B^{(2)} - S^{(2)}T^{(2)})/(AB - ST)^{(2)}]. \quad (5)$$

We shall denote by Δ the symmetry corresponding to root w_2,

$$\Delta(A,B,C,S,T) = (S,T,C + w_2,A,B). \quad (6)$$

Some properties of Δ are as follows.

(a) Δ is an involution, $\Delta^2 = 1$.

(b) The base points of Δ, that is, the points where Δ is not defined (giving homogeneous transformed coordinates all equal to zero), are the points canceling both the numerator and denominator of Eq. (5).

The base points can be obtained by making use (for $k = 2$) of the first part of the following identity:

$$(AB - ST)^{(k)} = \begin{cases} (A + S)^{(k)}(B + S)^{(k)}, & \text{if } A + B + S + T = k - 1, \\ (A + S - 1)^{(k-1)}(B + S - 1)^{(k-1)}((A + S)(B + S) - kS), & \text{if } A + B + S + T = k. \end{cases}$$

It turns out that the base points consist of the 18 three-spaces of Φ given in Table IV. The neighborhood of a base point is transformed by Δ into a line (i.e., when we let A, B, C, S, T approach a base point from all directions, the corresponding transforms by Δ tend to points forming a line). The neighborhoods of points in $E_{(13)(24)}$ are lines that generate $E_{(15)(46)}$, so we write $\Delta_N(E_{(13)(24)}) = E_{(15)(46)}$. We have a similar property for the 18 three-spaces of base points: $\Delta_N(E_{(25)(46)}) = E_{(13)(25)}$, $\Delta_N(E_{(13)(46)}) = E_{(13)(46)}, \ldots$, which is also displayed in Table IV.

(c) We know very little about the group of rational symmetries generated by Δ and the permutations of the x_i. We conjecture that this group is infinite. Calculating orbits of $\Delta_{13} = (13) \circ \Delta$ (Δ followed by the permutation of x_1 and x_3) in $P^5(F_p)$ (the five-dimensional projective space over the field F_p of integers modulo a prime number p), we get divisors (the number of points of an orbit) of the order k of Δ_{13} if this order is finite. By calculating a few orbits we got that if k exists, it is a multiple of a very large number ($> 10^{80}$).

IV. SOME CUBICS ON THE SURFACE Φ

If we put $S = A$ and $T = B$ in Eq. (1) we observe that Φ factorizes in three linear factors and one cubic factor,

$$\Phi = AB(A + B - 1)F_1,$$
$$F_1 = C^2 + 2(A + B - 1)C - (A - 1)(B - 1)(2A + 2B - 1). \quad (7)$$

A similar factorization also occurs by setting $S = A$ and $T = B + 1$,

$$\Phi = AB(A + B)F_2,$$
$$F_2 = C^2 + (2B + 1)C - (A - 1)(B + 1)(2A + 2B - 1). \quad (8)$$

The geometrical interpretation of these factorizations is very simple. For example, relations $S = A$ and $T = B$ define a projective subspace P_1 of $P^5(\mathbb{C})$ of dimension 3. Equation (7) describes the intersection of P_1 and Φ. The factorization means that this intersection consists of three planes and one cubic surface. The three planes are in fact, the intersections of P_1 with the three-spaces $E_{(23)(56)}$, $E_{(13)(46)}$, and $E_{(15)(24)}$. Similarly, Eq. (8) describes the intersection of the subspace P_2 ($S = A, T = B + 1$) with Φ that consists of three planes, intersections of P_2 with the three-spaces $E_{(23)(56)}$, $E_{(13)(25)}$, and $E_{(15)(36)}$, and of the cubic surface F_2 (we also denote by F_2 the surface of P_2 defined by the equation $F_2 = 0$).

In $P^5(\mathbb{C})$ the intersection of two projective subspaces of dimension 3 is, in general, a line. So the intersections of a generic projective subspace P of dimension 3 with the spaces $E_{(kl)(mn)}$ consist of lines. It is only for particular positions of P that some of the intersections of P with $E_{(kl)(mn)}$ become planes giving a factorization of linear factors in the equation of the intersection. It happens that there is an interesting family of such three-spaces:

$$P_a \begin{cases} x_1 + x_2 + x_3 + x_4 - a(x_1 + x_2) = 0, \\ x_2 + x_4 + a(x_3 + x_5) = 0. \end{cases} \quad (9)$$

The space P_a intersects each of the spaces $E_{(12)(34)}$, $E_{(13)(25)}$, and $E_{(24)(36)}$ along a plane. We can take any value

TABLE IV. The 18 three-spaces of base points of Δ. Two three-spaces on the same line in the first and second columns are exchanged by Δ_N. The three-spaces in the third column are self-transformed by Δ_N.

$E_{(13)(24)}$	$E_{(15)(46)}$	$E_{(13)(46)}$
$E_{(13)(25)}$	$E_{(25)(46)}$	$E_{(14)(25)}$
$E_{(13)(56)}$	$E_{(23)(46)}$	$E_{(14)(36)}$
$E_{(14)(23)}$	$E_{(14)(56)}$	$E_{(15)(24)}$
$E_{(15)(23)}$	$E_{(24)(56)}$	$E_{(23)(56)}$
$E_{(15)(36)}$	$E_{(24)(36)}$	$E_{(25)(36)}$

for a, excepted $a=0$ for which P_a coincides with $E_{(13)(24)}$, and $a=1$ for which P_a coincides with $E_{(34)(25)}$. Algebraically we use the projective coordinates u, v, w, and z of P_a:

$$
\begin{aligned}
x_1 &= u - v,\\
x_2 &= v,\\
x_3 &= (a-1)u + v - w,\\
x_4 &= -v + w,\\
x_5 &= (1-a)u - v + (1-1/a)w,\\
x_6 &= -u + v - (1-1/a)w + z.
\end{aligned}
$$

Substituting into Φ, we obtain a factorization of the form

$$\Phi = uv(au - v)F_a,$$

where F_a describes a cubic surface. Rather than writing the complicated expression of F_a in terms of u, v, w, and z we use the classical theory as exposed in Chap. VII of Semple and Roth[5] to obtain a simpler form. The cubic F_a has one double point only when $a=-1, \frac{1}{2}$, or 2. For these values of a, there is a permutation of the x_i coordinates such that the space P_a and the cubic F_a coincide with the space P_2 and the cubic F_2 of Eq. (8), respectively. For other values of a, F_a has no double point and possesses a system of 27 lines that are rational in a. There are 45 tritangent planes that are also rational in a and cut the cubic along three lines. The method for simplifying the equation of the cubic consists in finding a pair of associated Steiner trihedrals. This is two sets (X_1,X_2,X_3), (Y_1,Y_2,Y_3) of three tritangent planes (of equations $X_1=0$, $X_2=0$, ...) such that the mutual intersections as shown in the array

$$
\begin{array}{c} \\ Y_1 \\ Y_2 \\ Y_3 \end{array}
\begin{array}{c}
\begin{array}{ccc} X_1 & X_2 & X_3 \end{array} \\
\begin{pmatrix} l_1 & l_2 & l_3 \\ l_4 & l_5 & l_6 \\ l_7 & l_8 & l_9 \end{pmatrix}
\end{array}
$$

are nine different lines $l_1,\ldots,l_9$ of the cubic F_a. There are 120 such pairs of Steiner trihedrals, but it is enough to find one of these. It is then possible to choose $X_1, X_2, X_3, Y_1, Y_2, Y_3$ such that the equation of the cubic takes the form $X_1X_2X_3 = Y_1Y_2Y_3$ and such that the following relation is verified: $X_1 + X_2 + X_3 = Y_1 + Y_2 + Y_3$. Then by setting $X_1 = y_2 + y_3$, $X_2 = y_1 + y_3$, $X_3 = y_1 + y_2$, $Y_1 = -y_5 - y_6$, $Y_2 = -y_4 - y_6$, $Y_3 = -y_4 - y_5$ the equation of the cubic can be written as

$$
\det \begin{vmatrix} 0 & y_2+y_3 & y_5+y_6 \\ y_4+y_6 & 0 & y_1+y_3 \\ y_1+y_2 & y_4+y_5 & 0 \end{vmatrix} = 0 \tag{10}
$$

or as

$$\sum_{i=1}^{6} y_i^3 = 0. \tag{11}$$

Carrying out these calculations, we obtained that a possible choice for the y_i is given by

$$
\begin{aligned}
y_1 &= -(a-1)a^2u + (a-1)aw \\
&\quad + (a^3 - a^2/2 - 3a/2 + 1/2)z, \\
y_2 &= -(a-1)^2au + (a-1)^2w \\
&\quad + (a^3 - 5a^2/2 + a/2 + 1/2)z, \\
y_3 &= (a-1)a^2u - (a-1)^2w \\
&\quad - (a^3 - 3a^2/2 + 3a/2 - 1/2)z, \\
y_4 &= -(a-1)^2au - 2(a-1)av \\
&\quad + (a-1)aw + (a^2 + a - 1)z/2, \\
y_5 &= (a-1)^2au + 2(a-1)av \\
&\quad - (a-1)aw - (a^2 - 3a + 1)z/2, \\
y_6 &= (a-1)^2au - (a-1)aw \\
&\quad - (a^3 - 3a^2/2 - a/2 + 1/2)z.
\end{aligned} \tag{12}
$$

These variables are linked by two linear relations:

$$
\begin{aligned}
&\sum_{i=1}^{6} y_i = 0, \\
&2(a-1)y_1 - 2ay_2 - (a^2 - a + 1)(y_4 + y_5) = 0.
\end{aligned} \tag{13}
$$

The sum of cubes of y_i is then related to the cubic factor F_a by

$$\sum_{i=1}^{6} y_i^3 = 3(2a-1)(1-1/a)^3F_a,$$

so that for $a \neq \frac{1}{2}$ the equation of the cubic F_a is given by Eq. (10) or (11).

The cubic F_a can be parametrized rationally by homogeneous variables b, c, d by solving in terms of u, v, w the set of linear equations

$$
\begin{aligned}
& & (y_2+y_3)c & + (y_5+y_6)d & = 0, \\
(y_4+y_6)b & & & + (y_1+y_3)d & = 0, \\
(y_1+y_2)b & + (y_4+y_5)c & & & = 0.
\end{aligned} \tag{14}
$$

Indeed the equation of the cubic [Eq. (10)] is the result of eliminating b, c, and d from Eq. (14), and as shown in Semple and Roth[5] the correspondence between the projective plane b, c, d and the cubic F_a is birational (i.e., bijective and rational).

Dehomogenizing by $c=1$, for example, and $z=1$, we obtain six rational functions $R_i(a,b,c)$ that give the parametrization $x_i = R_i(a,b,d)$ of the cubic F_a for fixed a. We omit giving the complicated expressions of the R_i. We can interpret this result by considering the surface Q (of dimension 4) generated by the spaces P_a by varying a. The equation of Q is obtained by eliminating a from Eqs. (9),

$$
\begin{aligned}
&(x_1 + x_2 + x_3 + x_4)(x_3 + x_5) \\
&\quad + (x_1 + x_2)(x_2 + x_4) = 0,
\end{aligned}
$$

so that Q is a quadric. The functions R_i are thus giving a rational parametrization of the intersection of Q and Φ in terms of the three independent parameters a, b, and d.

The cubic F_1 can be studied by proceeding as in the case of cubic F_a. We introduce in this case the following y_i:

$$
\begin{aligned}
&y_1 = -\tfrac{3}{4}, \quad y_2 = -A - B - C + \tfrac{5}{4}, \\
&y_3 = A + B + C - \tfrac{3}{4}, \quad y_4 = B - \tfrac{1}{4}, \\
&y_5 = A - \tfrac{1}{4}, \quad y_6 = -A - B + \tfrac{3}{4},
\end{aligned}
$$

which are linked by

$$\sum_{i=1}^{6} y_i = 0 \tag{15}$$

and

$$2y_1 + 3(y_2 + y_3) = 0.$$

The expression F_1, Eq. (7) then takes the form

$$F_1 = \frac{2}{3} \sum_{i=1}^{6} y_i^3. \tag{16}$$

The cubic F_1 then can be parametrized by solving Eq. (14). This gives, setting $d = 1$ and $c = b^2 - a$, a full rational parametrization of F_1 as

$$\begin{aligned} A &= (b^4 + b^2 - 2b)/2a + a/2 - b^2, \\ B &= (b^2 - a + 1)/2, \\ C &= (b-1)A + 1 - (b^2 + b - a)/2. \end{aligned} \tag{17}$$

In the case of the cubic F_2 we define similarly

$$\begin{aligned} &y_1 = \tfrac{1}{4}, \quad y_2 = -B - C - \tfrac{1}{4}, \\ &y_3 = B + C + \tfrac{3}{4}, \quad y_4 = B + \tfrac{1}{4}, \\ &y_5 = A - \tfrac{5}{4}, \quad y_6 = -A - B + \tfrac{1}{4}, \end{aligned}$$

which are linked by

$$\sum_{i=1}^{6} y_i = 0$$

and (18)

$$3y_1 + y_4 + y_5 + y_6 = 0.$$

The expression F_2, Eq. (8), then takes the form

$$F_2 = \frac{2}{3} \sum_{i=1}^{6} y_i^3. \tag{19}$$

For the cubic F_2 there is a very simple way of obtaining a rational parametrization. We have already mentioned that F_2 has one double point Ω. It is $(A = 1, B = -\frac{1}{2}, C = 0)$. The line (for fixed a and b the line is parametrized by t),

$$A = a(2t-1) + 1, \quad B = t - 1, \quad C = b(2t-1), \tag{20}$$

intersects F_2 twice at Ω (for $t = \frac{1}{2}$) and at another point given by

$$t = b(b+1)/a(2a+1), \tag{21}$$

as can be verified by substituting Eq. (20) into F_2. Equations (20) and (21) give a rational parametrization of F_2 in terms of the two parameters a and b. Let us note that this method cannot be applied to F_1 or F_a, which have no double points.

It is clear that Eqs. (18) and (19) describing the cubic F_2 are invariant in the permutations of the triplet (y_4, y_5, y_6) and the pair (y_2, y_3). The corresponding symmetry expressed in terms of A, B, and C is described in Table V. In fact, the 12 transformations are the only projective transformations of P_2 that leave F_2 invariant. This can be shown by considering the system of Steiner trihedrals and the double point of F_2 that have to be invariant under any projective symmetry.

TABLE V. Symmetries of $F_2(A,B,C)$. The cubic polynomial F_2 takes the same value for the 12 sets of A, B, C.

A	B	C
A	B	$-2B - C - 1$
A	$-A - B$	$A - C - 1$
A	$-A - B$	$A + 2B + C$
$B + \frac{3}{2}$	$A - \frac{3}{2}$	$-A - B - C + \frac{1}{2}$
$B + \frac{3}{2}$	$A - \frac{3}{2}$	$-A + B + C + \frac{3}{2}$
$B + \frac{3}{2}$	$-A - B$	$A - C - 1$
$B + \frac{3}{2}$	$-A - B$	$A + 2B + C$
$-A - B + \frac{3}{2}$	$A - \frac{3}{2}$	$-A - B - C + \frac{1}{2}$
$-A - B + \frac{3}{2}$	$A - \frac{3}{2}$	$-A + B + C + \frac{3}{2}$
$-A - B + \frac{3}{2}$	B	$-2B - C - 1$
$-A - B + \frac{3}{2}$	B	C

Similarly, Eqs. (15) and (16) for the cubic F_1 are also invariant under the same 12 permutations of the y_i as in the case of F_2. However unlike the case of F_2, the corresponding transformations are simply permutations of the x_i coordinates.

V. CONCLUDING REMARKS

(1) It is still an open question whether there exists or not a full rational parametrization of the surface Φ (in terms of four independent parameters). The parametrizations that we have found (in terms of three or two independent parameters) really represent a very small part of the surface.

(2) Once a rational parametrization is found, one would like to know how to find all the values of the parameters that give genuine zeros of $6j$, that is, for which the corresponding A, B, C, S, T are integers $\geqslant 2$. This is, however, a difficult problem in itself, even for a simple parametrization like Eqs. (20) and (21) for the cubic F_2. Indeed, if it is quite easy to generate integer A, B, C [for example setting $b = a(2a+1)$, and taking any integer for parameter a, in Eqs. (20) and (21)], it seems difficult to characterize the parameters a and b that give integers A, B, C without calculating A, B, and C. Note that a and b are not necessarily integers (for example, $a = \frac{1}{3}$, $b = \frac{5}{3}$ give $A = 6$, $B = 7$, $C = 25$).

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On discrete Schrödinger equations and their two-component wave equation equivalents

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An approach to inverse scattering problems for discrete Schrödinger equations, which are discrete three-term recursions, is presented by systematically transforming them into discrete two-component wave-propagation equations. The wave-propagation equations permit the immediate application of certain computationally efficient and physically insightful "layer-peeling" algorithms for inverse scattering. The mapping of three-term recursions to two-component evolution equations is one to many, because the relation between the "potential" sequence parametrizing Schrödinger equations and the "reflection coefficient" sequence determining local wave interaction is a nonlinear difference equation. This mapping is examined in some detail and it is used to study both direct and inverse scattering problems associated with discrete Schrödinger equations.

I. INTRODUCTION

A highly nonstandard approach to the inverse scattering problem of quantum mechanics is due to Krein (see, e.g., Chadan and Sabatier,[1] p. 123). It is based on a transformation of the Schrödinger equation, parametrized by a potential function $P(x)$, into a two-component system of first-order differential equations parametrized by a local reflectivity function $K(x)$.

The point of this transformation is that the corresponding inverse scattering problem for the two-component system leads to an integral equation (the Krein equation) different from the classical equations due to Gel'fand and Levitan and to Marchenko. One can formally show in a rather straightforward way that, to a given one-dimensional second-order nonhomogeneous wave equation

$$\left(\frac{\partial}{\partial x^2}-\frac{\partial^2}{\partial t^2}\right)V(x,t)-P(x)V(x,t)=0 \tag{1.1}$$

(which by Fourier transforming w.r.t. the time variable becomes a Schrödinger equation), we can associate a two-component first-order differential equation [relating right and left propagating waves $\{W_R(x,t),W_L(x,t)\}$] of the following form:

$$\frac{\partial}{\partial x}\begin{bmatrix}W_R(x,t)\\W_L(x,t)\end{bmatrix}=\begin{bmatrix}-\partial/\partial t & -K(x)\\-K(x) & \partial/\partial t\end{bmatrix}\begin{bmatrix}W_R(x,t)\\W_L(x,t)\end{bmatrix}. \tag{1.2}$$

Indeed, if the reflectivity function $K(x)$ is related to the potential $P(x)$ via the Riccati equation

$$-\frac{d}{dx}K(x)+K^2(x)=P(x) \tag{1.3}$$

and $V(x_0,t)=W_R(x_0,t)+W_L(x_0,t)$ at some point x_0, it follows that

$$V(x,t)=W_R(x,t)+W_L(x,t) \tag{1.4}$$

holds everywhere (see Chadan and Sabatier,[1] Bruckstein and Kailath,[2] and Bruckstein, Levy, and Kailath[3]). Note that if one starts with wave-propagation equations as in (1.2), then it is immediate to determine the potential function of the corresponding second-order (Schrödinger) equation; however, the reverse mapping is more problematic. From (1.3) we expect it to be nonunique, since we also need an initial condition, say $K(x_0)$, in order to determine $K(x)$ given the potential $P(x)$.

Several interesting questions now arise in the context of Krein's approach to inverse scattering: For which potentials can we find reflectivity functions obeying (1.3)? Are there potentials for which the reflectivity function is uniquely determined from the corresponding Riccati equation? Are there potentials for which no reflectivity function obeying (1.3) exists? The answer obviously depends on the interval over which we wish to determine a model as well as on the properties of the potential $P(x)$. If the potential is identically 0 for $x\in[0,\infty)$ then reflectivity functions obeying (1.3) are of the form $K(0)/(1-K(0)x)$, and, to be well defined on the positive axis, $K(0)$ can be *any* negative value. However, had we required a solution over the entire real axis, the conclusion would have been that $K(x)=0$ is the only one that does not blow up at any point. This simple example shows that the mapping from potentials to reflectivity functions may sometimes be problematic.

We shall analyze the problems raised above for a discrete version of the wave (or Schrödinger) equation. Doing a straightforward discretization of Eq. (1.1), with both spatial and temporal quantization intervals chosen to have length Δ, one arrives at the equation

$$V(x+\Delta,t)+V(x-\Delta,t)=G(x)\{D+D^{-1}\}V(x,t)+O(\Delta^4), \tag{1.5}$$

where $G(x)$ is defined as

$$G(x)=\exp\{\Delta^2[P(x)/2]\} \tag{1.6}$$

and D acts on time sequences as a Δ/unit delay operator, i.e.,

$$Df(t)=f(t-\Delta) \quad \text{and} \quad D^{-1}f(t)=f(t+\Delta). \tag{1.7}$$

For details of the discretization see, e.g., Case and Kac.[4] If, for integer values of n and τ, $V(n\Delta,\tau\Delta)$ is rewritten as

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$V(n,\tau)$ and all functions of the (discrete) time index are replaced by formal two-sided power series in D, i.e.,

$$f(\tau) \to f(D) = \sum_{\tau \in Z} f(\tau) D^{\tau},$$

Eq. (1.5) becomes a discrete wave equation

$$V(n+1,D) + V(n-1,D) = G(n)\{D + D^{-1}\}V(n,D), \tag{1.8}$$

which has the form of a "classical" discrete Schrödinger equation with eigenvalue $2\lambda = D + D^{-1}$ (see, e.g., Case and Kac[4] and Case[5]). Note that by (1.6) the potential sequence $G(n)$ is always positive. Since in the continuous case it is assumed that $P(x)$ tends to 0 as x goes to infinity (in each direction), we have that $G(n)$ tends to 1 as $|n| \to \infty$. It is usually further assumed that convergence to these limits is quite fast, therefore our discussion will often refer to the case of $G(n) = 1$ for $|n|$ exceeding a certain value N.

We shall also consider here a generalized version of (1.8) parametrized by two sequences of numbers $\{F(n),G(n)\}$,

$$F(n)V(n+1,D) + F(n-1)V(n-1,D) = G(n)\{D + D^{-1}\}V(n,D), \tag{1.9}$$

where $F(n)$ is never zero and tends to 1 as $|n| \to \infty$.

Our interest in discrete Schrödinger equations arose from recent research on efficient algorithms for solving nested (linear) systems of equations, or integral equations, recursively for increasing dimensions. Such algorithms provide lattice filter solutions for linear prediction/estimation of stochastic processes and are of crucial importance in digital signal processing (see, e.g., the discussion in Kailath[6] and the references therein). It gradually became clear that there are close connections between inverse scattering problems for transmission-line models and estimation theory, and in both fields the problems are solved once one has an algorithm for recursively determining a layered medium, or a cascade filter, from impulse responses or equivalent spectral data. Moreover, in both fields the solutions may be found either by first deriving and solving sets of linear equations (or integral equations, in the continuous case) or in a direct way, by exploiting the causality of signal propagation and structure of the layered medium, i.e., the assumed structure of the elementary processors in a cascade filter. This research also showed that the more efficient way of finding the solution of inverse scattering problems is via a recursive layer identification and peeling process, in which signals are propagated through the already identified layers to provide the scattering data for the deeper and yet unidentified layers of the medium (see, e.g., Bruckstein, Levy, and Kailath[3] and Bruckstein and Kailath[2,7]). It was thus natural to look for similar algorithmic solutions to the classical inverse scattering problem, which starts with the Schrödinger equation as the propagation model. This paper shows that, in the discrete case previously analyzed by Case and Kac,[4] and Case[5,8] and several others, direct layer-peeling solutions are always possible via a mapping of the Schrödinger equation to a two-component wave-propagation model, and hence to an equivalent discrete transmission line. The mapping then provides a new algorithmic inverse scattering procedure that does not proceed via classical systems of equations (see, e.g., Case[5]) corresponding to the solutions of Gel'fand–Levitan, Marchenko, or Krein (see, e.g., Chadan and Sabatier[1]).

This paper is organized as follows. The next section deals with the formal mapping of the discrete Schrödinger equation into a two-term wave evolution equation, and proves that such a mapping is always possible. In Sec. III we then discuss some properties of the mapping between potentials and the reflection coefficients that parametrize two-term evolution equations. In Sec. IV we deal with direct and inverse scattering problems and derive layer-peeling algorithms for inverse scattering based on inverse scattering for transmission-line models; an example from Case[5] is then reexamined from this point of view.

II. FROM THREE-TERM TO TWO-COMPONENT EQUATIONS

Equations (1.8) and (1.9) relate discrete functions of *time*, in their formal power series representations, at three consecutive points in *space*. They may be regarded as recursive ways of defining $V(n,D)$, given the "interaction" parameters $\{F(\cdot),G(\cdot)\}$ and some initial conditions $V(0,D)$ and $V(1,D)$, say.

Suppose that, over a certain interval in the space coordinate $n \in [N_L,N_R]$, we have $F(n) = 1$ and $G(n) = 1$. It is then straightforward to verify that, over $[N_L,N_R]$, the solution of the three-term recursion is of the form

$$V(n,D) = D^{n}\phi_R(D) + D^{-n}\phi_L(D). \tag{2.1}$$

To determine the functions $\phi_{R,L}(D)$ we of course need the signals $V(n,D)$ at two points in space. In the time domain, (2.1) means that

$$V(n,\tau) = \phi_R(\tau - n) + \phi_L(\tau + n), \tag{2.2}$$

i.e., $V(n,\tau)$ is a sum of two *noninteracting* right and left propagating waves over $n \in [N_L,N_R]$. Regarding $V(n,\tau)$ as a sum of waves propagating in opposite directions can give simple physical interpretations to relations induced between time signals at various points in space, as a consequence of linear and *causal* wave interaction. One of the major aims of this paper is to show that a decomposition of signals $V(n,\tau)$ into *interacting* waves propagating in opposite directions can be done in general: The potential sequences $\{F(n),G(n)\}$ determine the local interactions between the right and left propagating wave components of $V(n,\tau)$ via a local *reflection coefficient sequence* $\{K_n\}$, corresponding to the continuous reflectivity function.

To do this, we start by writing, for a general Schrödinger equation, that $V(n,D)$ is the sum of two components as follows:

$$V(n,D) = [1 \;\; 1]\begin{bmatrix} W_R(n,D) \\ W_L(n,D) \end{bmatrix}. \tag{2.3}$$

Now, since $V(n,D)$ obeys (1.8) or (1.9), we have to determine a sequence of operators, $\{\Theta(n,D)\}$, that will yield wave components at $n+1$ from the ones at n, and also ensure that (2.3) will hold at all points in space. This sequence of 2×2 matrix operators will, of course, be determined by

the potential sequences, i.e., $G(n)$ and $F(n)$, that parametrize the three-term evolution equation. Since we wish to consider both forward and backward evolution operators we require the $\Theta(n,D)$ to be invertible for every n. Writing

$$\begin{bmatrix} W_R(n+1,D) \\ W_L(n+1,D) \end{bmatrix} = \Theta(n,D) \begin{bmatrix} W_R(n,D) \\ W_L(n,D) \end{bmatrix}, \tag{2.4}$$

some algebra shows that we can determine $V(n+1,D)$ from $V(n,D)$ and $V(n-1,D)$ as follows. Here $V(n+1,D)$ is given by

$$V(n+1,D) = [1\ \ 1]\Theta(n,D) \begin{bmatrix} W_R(n,D) \\ W_L(n,D) \end{bmatrix} \tag{2.5}$$

and using (2.4) and (2.5) we also have

$$\begin{bmatrix} V(n,D) \\ V(n-1,D) \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ [1\ \ 1]\Theta^{-1}(n-1,D) \end{bmatrix} \begin{bmatrix} W_R(n,D) \\ W_L(n,D) \end{bmatrix}. \tag{2.6}$$

This yields

$$V(n+1,D) = [1\ \ 1]\Theta(n,D) \begin{bmatrix} 1 & 1 \\ [1\ \ 1]\Theta^{-1}(n-1,D) \end{bmatrix}^{-1} \times \begin{bmatrix} V(n,D) \\ V(n-1,D) \end{bmatrix}, \tag{2.7}$$

a three-term recursion for $V(n,D)$ that should be made identical to (1.9). For this the sequence of matrices $\Theta(n,D)$ must obey

$$[1\ \ 1][\Theta(n,D)] = \left[\frac{G(n)}{F(n)}\{D + D^{-1}\} - \frac{F(n-1)}{F(n)}\right] \times \begin{bmatrix} 1 & 1 \\ [1\ \ 1]\Theta^{-1}(n-1,D) \end{bmatrix}. \tag{2.8}$$

If we set

$$\Theta(n,D) = \begin{bmatrix} \theta_{11}(n,D) & \theta_{12}(n,D) \\ \theta_{21}(n,D) & \theta_{22}(n,D) \end{bmatrix}, \tag{2.9}$$

then (2.8) reads

$$[\theta_{11}(n,D) + \theta_{21}(n,D) \quad \theta_{12}(n,D) + \theta_{22}(n,D)] = \left[\frac{G(n)}{F(n)}\{D + D^{-1}\} - \frac{F(n-1)}{F(n)}\right] \begin{bmatrix} 1 & 1 \\ \dfrac{\theta_{22}(n-1,D) - \theta_{21}(n-1,D)}{\det \Theta((n-1,D)} & \dfrac{\theta_{11}(n-1,D) - \theta_{12}(n-1,D)}{\det \Theta(n-1,D)} \end{bmatrix}. \tag{2.10}$$

There are many ways of choosing operator sequences that will make (2.10) into an identity. We shall be interested, for reasons to become clear soon, in nonsingular matrices having the following structure:

$$\Theta(n,D) = \Theta_n \begin{bmatrix} D & 0 \\ 0 & D^{-1} \end{bmatrix} = \gamma_n \begin{bmatrix} 1 & -K_n \\ -K_n & 1 \end{bmatrix} \begin{bmatrix} D & 0 \\ 0 & D^{-1} \end{bmatrix}, \tag{2.11}$$

where we require $|K_n| \neq 1$, for all n. Thus it will be assumed that the propagation operators are composed of a relative shift operator, delaying $W_R(n,D)$ one unit of time and advancing $W_L(n,D)$ by the same amount, followed by a *symmetric* pure-gain matrix mixing the two sequences, $DW_R(n,D)$ and $D^{-1}W_L(n,D)$, pointwise in time. We assume this form for the operators $\Theta(n,D)$ because their so-called scattering domain representation $\Sigma(n,D)$, relating $W_R(n+1,D)$ and $W_L(n,D)$ to $W_R(n,D)$ and $W_L(n+1,D)$, is then the cascade connection of a causal scattering matrix that delays the waves propagating in opposite directions and a wave-interaction matrix that transmits part of the signal and reflects part of it adding the reflected part to the wave propagating in the opposite direction (see Fig. 1). Indeed, writing

$$\begin{bmatrix} W_R(n+1,D) \\ W_L(n,D) \end{bmatrix} = \Sigma(n,D) \begin{bmatrix} W_R(n,D) \\ W_L(n+1,D) \end{bmatrix} \tag{2.12}$$

a few steps of algebra show [using (2.11)] that

$$\Sigma(n,D) = \begin{bmatrix} 1 & 0 \\ 0 & D \end{bmatrix} \times \begin{bmatrix} (\gamma_n^2 - K_n^2)1/\gamma_n & -K_n \\ K_n & 1/\gamma_n \end{bmatrix} \begin{bmatrix} D & 0 \\ 0 & 1 \end{bmatrix}. \tag{2.13}$$

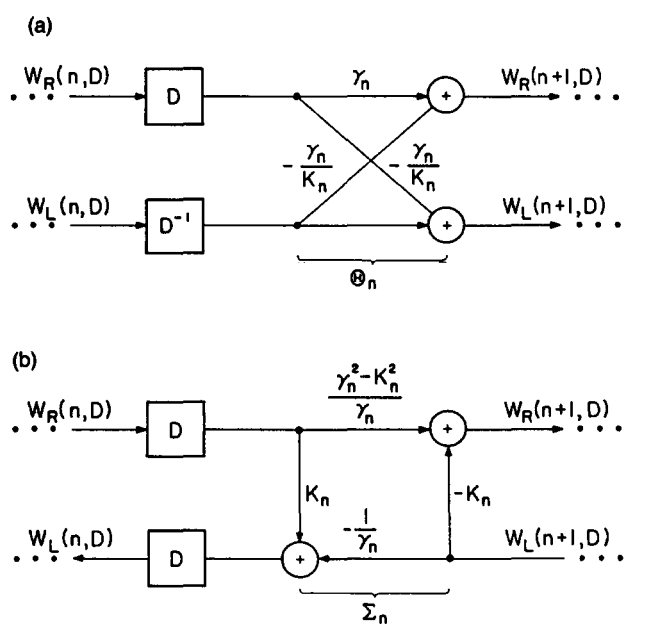

FIG. 1. (a) Transmission and (b) scattering representations of wave-propagation operators.

The above assumed structure for the signal transfer operators, and their scattering equivalents, leads to transmission-line models that are discrete-case analogs of (1.2), see, e.g., Bruckstein and Kailath.[7]

Using (2.11) for the $\Theta(n,D)$ operators (2.10) becomes

$$[\gamma_n(1-K_n)D \quad \gamma_n(1-K_n)D^{-1}] = \left[\frac{G(n)}{F(n)}\{D+D^{-1}\} - \frac{F(n-1)}{F(n)}\right]\begin{bmatrix} \dfrac{1}{D^{-1}\gamma_{n-1}^{-1}+D\gamma_{n-1}^{-1}K_{n-1}} & \dfrac{1}{D^{-1}\gamma_{n-1}^{-1}K_{n-1}+D\gamma_{n-1}^{-1}} \\ 1-K_{n-1}^2 & 1-K_{n-1}^2 \end{bmatrix} \tag{2.14}$$

and the equation becomes an identity provided

$$\gamma_n = F(n)/G(n+1)(1-K_n^2)\,, \tag{2.15a}$$

$$(1+K_n)(1-K_{n-1}) = F^2(n)/G(n)G(n+1)\,. \tag{2.15b}$$

Here we have used the fact that delay and advance operators commute with scalar gains and have equated the coefficients of D and D^{-1} in (2.14). Thus to have that $V(n,D) = W_R(n,D) + W_L(n,D)$, the wave components should evolve according to (2.4) with the parameters of the symmetric delay-and-interaction operators $\Theta(n,D)$ being determined by (2.15).

To summarize, suppose that we are dealing with a three-term recursion (1.9) defined over $n\in(-\infty,\infty)$. Given the potential sequences $\{F(n),G(n)\}$, we have the following result: If a sequence K_n can be determined so that it obeys (2.15b) and is, for all n, different in absolute value from 1, then we can associate to the three term recursion (1.9) the following transmission-line type wave propagation model

$$\begin{bmatrix} W_R(n+1,D) \\ W_L(n+1,D) \end{bmatrix} = \frac{F(n)}{G(n+1)(1-K_n^2)}\begin{bmatrix} 1 & -K_n \\ -K_n & 1 \end{bmatrix} \times \begin{bmatrix} D & 0 \\ 0 & D^{-1} \end{bmatrix}\begin{bmatrix} W_R(n,D) \\ W_L(n,D) \end{bmatrix}. \tag{2.16}$$

We now show that we can always determine infinite sequences K_n, so that $|K_n|\neq 1$ for all n, and also satisfying (2.15b). Let us further analyze the relation (2.15b). Define the strictly positive sequence of numbers

$$\rho_n = F^2(n)/G(n)G(n+1)\,. \tag{2.17}$$

It is clear that the nonlinear difference equation (2.15b) can be read either as a right, or forward propagating recursion, yielding K_n from K_{n-1},

$$K_n = \rho_n/(1+K_{n-1}) - 1\,, \tag{2.18a}$$

or as a left, or backward propagation equation, yielding K_n from K_{n-1},

$$K_{n-1} = 1 - \rho_n/(1+K_n)\,. \tag{2.18b}$$

To determine a $\{K_n\}$ sequence, we thus need to choose an "anchoring" value at some point, say $n=0$, i.e., to set an initial condition to the forward and backward recursions (2.18). Clearly we need to have K_n different from 1 in absolute value, since ρ_n in (2.15b) is strictly positive. The following lemma shows that we can *always* choose an initial condition that determines a $\{K_n\}$ sequence that has $|K_n|\neq 1$ for all n.

Lemma: Given an arbitrary sequence of numbers $\{\rho_n\}$, $\rho_n > 0$ for all $n\in Z$, there exist uncountably many sequences $\{K_n\}$, such that, for all n,

$$(1+K_n)(1-K_{n-1}) = \rho_n\,.$$

Proof: We shall show that there are uncountably many values for K_0 for which both forward and backward recursions yield sequences K_n having $|K_n|\neq 1$. The forward recursions will never yield a -1 since ρ_n is always positive, however, they cannot be propagated past a point where the K-sequence hits a value of 1. The backward recursions never hit the value 1, however, they may at some point yield a -1, beyond which we cannot proceed. Assume that at all points $n>0$ we start backward recursions, i.e., (2.18b), with the initial value of 1, and at all points $n<0$ we start forward recursions with $K_n = -1$. We proceed, if it is possible, with these recursions until n reaches 0 and exclude the values that are attained at this point from the set of possible anchoring values for K_0. But, since any real value can be an anchor point for K_0 and the above described process rules out at most countably many of them, it will be possible to find uncountably many initial values K_0 that will yield solutions of the nonlinear difference equation (2.15b) on the entire line. Hence there always exist infinitely many different $\{K_n\}$ sequences that correspond to any given ρ_n sequence. Q.E.D.

We have proved that to any three-term recursion of the form (1.9) there correspond many wave propagation models of the form (2.16). We call these models wave-propagation equations because, as pointed out above, (2.16) implies that the signals $W_R(n,D)$ and $W_L(n,D)$ may indeed be regarded as waves propagating in opposite directions in a layered scattering medium that determines their causal interaction. The wave-interaction $\Sigma(n,D)$ show that the medium layers operate causally on the incoming waves $W_R(n,D)$ and $W_L(n+1,D)$ to generate the outgoing waves $W_R(n+1,D)$ and $W_L(n,D)$. As we see from (2.13) the pointwise interaction matrix of the layers' scattering representations have as right and left reflection gains K_n and $-K_n$, respectively. This is the reason for calling the K_n's local reflection coefficients.

The causal picture of wave propagation proves to be a most intuitive physical interpretation of signal interactions

described by the discrete Schrödinger equation: Given a potential sequence $\{G(n)\}$, or generally, a pair of sequences $\{F(n),G(n)\}$ we shall investigate the properties of the discrete Schrödinger equation via corresponding reflection coefficient sequences $\{K_n\}$.

III. POTENTIALS AND LOCAL REFLECTION COEFFICIENTS

It is usually assumed that the sequences $\{F(n),G(n)\}$ tend to 1 as $|n|\to\infty$. In this case the corresponding ρ_n sequences defined by (2.17) also converge to 1 with increasing $|n|$. We have from the forwards and backwards recursions (2.18) that, if K_n tends to a limit, then

$$\lim_{|n|\to\infty} K_n = 0 . \tag{3.1}$$

However, the convergence of K_n to 0 is conditioned on the asymptotic behavior of the sequence ρ_n. From (2.15) we see that, in order to have a convergent K_n sequence for $|n|\to\infty$, it is necessary that $\rho_n - 1$ approaches 0 as fast as $K_n - K_{n-1} - K_nK_{n-1}$ $(=\rho_n - 1)$, for some K_n sequence convergent to 0. It is not difficult to show that a sufficient condition for having a convergent K_n sequence is that $\delta_n = 1-\rho_n$ approaches 0 from above, i.e., so that $\rho_n < 1$ for all n big enough in their absolute value. This means, for example, that the potential in Eq. (1.8), $G(n)$, should obey $G(n)G(n+1) > 1$ for all n, a condition trivially met if $G(n)$ is always greater than 1.

To avoid dealing with convergence conditions we often assume that the potentials are already at their limiting value, 1, for $|n| > N_0$. In this case the iteration of the functions

$$\mathbf{F}_f(x) = 1/(1-x) - 1 \quad \text{and} \quad \mathbf{F}_b(x) = 1 - 1/(1-x) \tag{3.2}$$

yields K_n sequences that converge to 0 as $1/|n|$. To see this we can either check directly that sequences converging to 0 as $1/|n|$ satisfy the recursions induced by (3.2) or transform (2.18) into two-component recursions for A_n and B_n, where

$$K_n = A_n/B_n . \tag{3.3}$$

It is straightforward to show that

$$\begin{bmatrix} A_n \\ B_n \end{bmatrix} = \begin{bmatrix} 1 & \rho_n - 1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} A_{n-1} \\ B_{n-1} \end{bmatrix} \tag{3.4}$$

implying that, for $n > 0$, A_n and B_n are given by

$$\begin{bmatrix} A_n \\ B_n \end{bmatrix} = \prod_{i=n}^{0} \begin{bmatrix} 1 & \rho_i - 1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} K_0 \\ 1 \end{bmatrix} . \tag{3.5}$$

Now if $\rho_n = 1$ for $n > N_0$ we obtain

$$K_n = A_{N_0}/-(n-N_0)A_{N_0} + B_{N_0} \to 0 . \tag{3.6}$$

and a similar exercise shows that for $n\to -\infty$, K_n also tends to zero as $1/(|n-N_0|)$.

Note that if we had $F(n) = G(n) = 1$ for all $n\in Z$, the sequences K_n that would correspond to an anchoring value of K_0 would be

$$K_n = K_0/(1-nK_0) , \tag{3.7}$$

the excluded values for K_0 being $\{1/n | n\in Z\}$.

A. Conditions for losslessness

Suppose that we can find a sequence K_n corresponding to the given potential sequence(s) so that

$$|K_n| < 1 \quad \text{for all } n . \tag{3.8}$$

The evolution equations (2.16) into which the three-term recursion (1.9) is mapped then yield sequences proportional to those provided by the following associated wave equation:

$$\begin{bmatrix} W_R^*(n+1,D) \\ W_L^*(n+1,D) \end{bmatrix} = \frac{1}{(1-K_n^2)^{1/2}} \begin{bmatrix} 1 & -K_n \\ -K_n & 1 \end{bmatrix} \times \begin{bmatrix} D & 0 \\ 0 & D^{-1} \end{bmatrix} \begin{bmatrix} W_R^*(n,D) \\ W_L^*(n,D) \end{bmatrix} . \tag{3.9}$$

These equations describe wave propagation on a lossless transmission line, as discussed in Bruckstein and Kailath.[7] The interaction (gain) matrices are J lossless in the transmision representation, i.e.,

$$\Theta_n^* J \Theta_n^{*T} = J \quad \text{with } J = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{3.10}$$

and this implies that they are unitary (lossless) in their scattering representation.

Let us determine conditions under which a given three-term recursion may be mapped into a lossless model, with all reflection coefficients less than 1 in absolute value. From (2.19) we see that necessary conditions for this are

$$0 < \rho_n < 4 = \max\{(1+K_n)(1-K_{n-1})\} . \tag{3.11}$$

To obtain sufficient conditions, too, let us study the forward and backward recursions providing the $\{K_n\}$ sequence from the anchoring point K_0, say. A simple analysis of functions of the form

$$\mathbf{F}_f(x;\rho) = \rho/(1-x) - 1 \text{ and } \mathbf{F}_b(x;\rho) = 1 - \rho/(1+x) \tag{3.12}$$

shows that, if $\rho < 1$, then $\mathbf{F}_f(x;\rho)$ maps the interval $(-1,0)$ into itself, whereas $\mathbf{F}_b(x;\rho)$ maps $(0,1)$ into itself. If we therefore ensure that K_1 is in $(-1,0)$, then $K_n\in(-1,0)$ for all positive n, and similarly if $K_{-1}\in(0,1)$ then K_n will remain in that interval for all $n < 0$. Thus, choosing $K_0 = 0$ [or any value in the interval $(\rho_0 - 1, 1-\rho_1)$], we shall have that $|K_n| < 1$ for all n, provided $\rho_n < 1$, for all n. This proves that *a sufficient condition for the three-term recursion (1.9) to correspond to a lossless two-component evolution equation is that all the positive values ρ_n, defined by (2.17), are less than 1 in magnitude.*

In the special case of the three-term recursion (1.8), which is parametrized by the single sequence $\{G(n)\}$, we realize that the above condition for losslessness is satisfied automatically provided we have all $G(n) > 1$. This corresponds to a continuous model for which the potential is always positive, a well-known condition for the nonexistence of so-called "bound-state" solutions for Schrödinger equations. Losslessness should intuitively correspond to no-bound-state situations, since bound states correspond to energy trapped in the medium, which is impossible in lossless

media (see, e.g., Ablowitz and Segur[9]).

B. Local mapping between reflection coefficients and potentials

Suppose we are given a local reflection coefficient sequence $\{K_n\}$ and we ask for the potential sequences $\{F(n),G(n)\}$. These sequences should obey

$$F^2(n)/G(n)G(n+1) = \rho_n = (1+K_n)(1-K_{n-1}) \tag{3.13}$$

and they are not uniquely determined by (3.13). If $F(n)=1$ for all n and $G^*(n)$ obeys the relation (3.13), then clearly $G(n) = G^*(n)Z^{(-1)^*}$ is another valid potential sequence for any $Z \neq 0$. To determine the potential sequence uniquely we need to anchor it at a given point, say $n=0$. Suppose, however, that we wish to have a local functional dependence of the potentials on the reflection coefficients. If we try to set $G(n) = \Gamma(K_{n-1})$, then we see that it is necessary for $F(n)$ to be different from 1. Writing (3.13) out in terms of the $\Gamma(K_n)$ we obtain

$$F^2(n) = (1+K_n)\Gamma(K_n)(1-K_{n-1})\Gamma(K_{n-1}) . \tag{3.14}$$

Requiring further $F(n)$ to be independent of K_{n-1} leads to

$$\Gamma(K_{n-1}) = G(n) = 1/(1-K_{n-1}) \tag{3.15}$$

and

$$F(n) = [(1+K_n)/(1-K_n)]^{-1/2}$$

and we see that, to have positive $G(n)$ and real $F(n)$, it is necessary for all K_n to be less than unity in magnitude. In this case the evolution equations (2.16) become identical to the lossless propagation model (3.9). Three-term recursions having $F(n)$ and $G(n)$ given by (3.15) were first derived in (Bruckstein and Kailath[2]) from the corresponding lossless two-component equations as recursions that describe the evolution of the *voltage* on a transmission line with piecewise constant impedance function. The associated *current* signals are defined as $I(n,D) = W_R(n,D) - W_L(n,D)$, and obey a complementary pair of three-term recursions, with $G(n)$ replaced by $\tilde{G}(n) = 1/[1+K_n]$.

We note that associated *wave difference* or current variables can be defined for arbitrary three-term recursions and then we can write that

$$\begin{bmatrix} V(n,D) \\ I(n,D) \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} W_R(n,D) \\ W_L(n,D) \end{bmatrix} \tag{3.16}$$

and we readily obtain two-component evolution equations of the following form:

$$\begin{bmatrix} V(n+1,D) \\ I(n+1,D) \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \times \Theta(n,D) \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} V(n,D) \\ I(n,D) \end{bmatrix} . \tag{3.17}$$

After some simple algebraic manipulation these equations can be put in the form

$$\begin{bmatrix} V(n+1,D) \\ I(n+1,D) \end{bmatrix} = \frac{F(n)}{2G(n+1)[1+K_n]} \begin{bmatrix} 1 & 0 \\ 0 & (1+K_n)/(1-K_n) \end{bmatrix} \times \begin{bmatrix} D+D^{-1} & D-D^{-1} \\ D-D^{-1} & D+D^{-1} \end{bmatrix} \begin{bmatrix} V(n,D) \\ I(n,D) \end{bmatrix} . \tag{3.18}$$

This form of two-component equations associated to a transmission-line model was recently found useful in deriving new and computationally efficient algorithms for matrix factorization and estimation applications. It turns out that, by parametrizing the media in terms of $\lambda_n = (1+K_n)/(1-K_n)$, these algorithms require about half the number of multiplications when compared to conventional transmission line based algorithms see, e.g., Bistritz, Lev-Ari, and Kailath.[10]

IV. DIRECT AND INVERSE SCATTERING PROBLEMS

Up to this point we discussed the basic three-term recursions (1.18) and (1.9) and showed that we can always associate to them two-component propagation equations of the form (2.16) or (3.18). The basic three-term recursions (1.9) can be written out in the space-time coordinates (n,τ) as a second-order system of partial linear difference equations (see, e.g., Fort,[11])

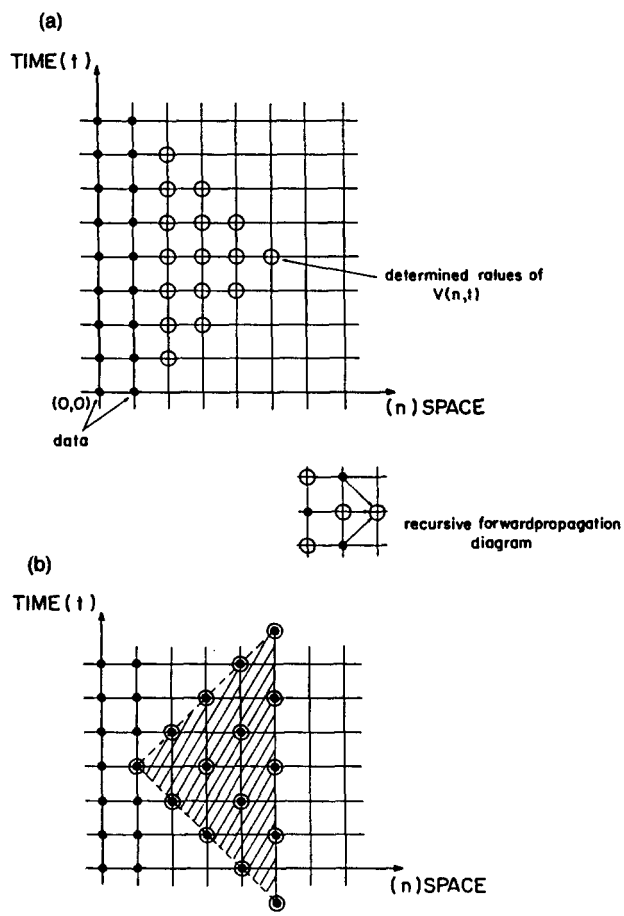

FIG. 2. (a) Computable regions of $V(n,\tau)$ from given sequences, and (b) a diagram of influence propagation from a certain data point.

$$a_r(n,\tau)V(n+1,\tau)+a_l(n,\tau)V(n-1,\tau)+a_u(n,\tau)V(n,\tau+1)+a_d(n,\tau)V(n,\tau-1)+a_c(n,\tau)V(n,\tau)=0\,, \tag{4.1}$$

where

$$a_r(n,\tau)=F(n+1)\,,\quad a_l(n,\tau)=F(n)\,,\quad a_u(n,\tau)=a_d(n,\tau)=-G(n)\,,\quad a_c(n,\tau)=0\,. \tag{4.2}$$

Notice that the $a_*(n,\tau)$ are independent of the time index τ, which made possible the transform analysis, i.e., the representation of (4.1) as a recursion relating formal power series via three-term propagation equations having constants or time-delay/advance operators as coefficients.

To determine $V(n,\tau)$ from (4.1), or the three-term recursions (1.9), we need to be given two initial condition sequences, say $V(0,\tau)$ and $V(1,\tau)$, or in general any pair $V(m,\tau)V(m+1,\tau)$. Then we can forwards or backwards propagate the three-term recursion to obtain the time sequence $V(n,\tau)$ at any point in space n. Furthermore, the sequence at $V(n,\tau)$ depends linearly on the initial given initial sequences. To analyze graphically the influence propagation of given data sequences we can plot space-time diagrams as depicted in Fig. 2. We see in these diagrams that given a contiguous portion of the data sequences, it will be possible to determine $V(n,\tau)$ in a certain influence region that can readily be mapped.

If we pass to the equivalent two-component domain, where we are given interlocked recursions for the right and left propagating signals then we need as initial conditions the two wave components at a certain point in space, say $W_R(m,\tau)$ and $W_L(m,\tau)$. The waves at any point in space will obviously be given by (in the transform domain),

$$\begin{bmatrix}W_R(n,D)\\W_L(n,D)\end{bmatrix}=M(m{:}n,D)\begin{bmatrix}W_R(m,D)\\W_L(m,D)\end{bmatrix}, \tag{4.3}$$

where the operator $M(m{:}n,D)$ is given by

$$M(m{:}n,D)=\begin{cases}[M_m^n(D)]=\displaystyle\prod_{i=n-1}^{m}\frac{F(i)}{G(i+1)[1-K_i^2]}\begin{bmatrix}1&-K_i\\-K_i&1\end{bmatrix}\begin{bmatrix}D&0\\0&D^{-1}\end{bmatrix}, & \text{if } n>m\,,\\ [M_n^m(D)]^{-1}=\displaystyle\prod_{i=m-1}^{n}\frac{G(i+1)}{F(i)}\begin{bmatrix}D^{-1}&0\\0&D\end{bmatrix}\begin{bmatrix}1&K_i\\K_i&1\end{bmatrix}, & \text{if } n<m\,.\end{cases} \tag{4.4}$$

Given a legal choice of "anchor" value for the reflection coefficient sequence, at m, K_m, and the data pair $\{V(m,D),V(m+1,D)\}$, we can determine the wave components $\{W_R(m,D),W_L(m,D)\}$ from

$$W_R(m,D)+W_L(m,D)=V(m,D)\,,\qquad \{F(m)/G(m+1)[1+K_m]\}(DW_R(m,D)+D^{-1}W_L(m,D))=V(m+1,D)\,, \tag{4.5}$$

i.e., we have

$$\begin{bmatrix}W_R(m,D)\\W_L(m,D)\end{bmatrix}=E(m,D)\begin{bmatrix}V(m,D)\\V(m+1,D)\end{bmatrix}=\begin{bmatrix}1&1\\\dfrac{F(m)}{G(m+1)[1+K_m]}D&\dfrac{F(m)}{G(m+1)[1+K_m]}D^{-1}\end{bmatrix}^{-1}\begin{bmatrix}V(m,D)\\V(m+1,D)\end{bmatrix}. \tag{4.6}$$

Now to determine $V(n,D)$ for any n we can write that

$$V(n,D)=[1\ \ 1]\begin{bmatrix}W_R(n,D)\\W_L(n,D)\end{bmatrix}=[1\ \ 1]M(m{:}n,D)E(m,D)\begin{bmatrix}V(m,D)\\V(m+1,D)\end{bmatrix} \tag{4.7}$$

and, since the choice of the reflection coefficient sequence, and thus of K_m, clearly does not enter in the determination of $V(n,D)$ from the initial conditions $\{V(m,D),V(m+1,D)\}$, we have that the row vectors

$$[\Phi(m{:}n,D)\Psi(m{:}n,D)]=[1\ \ 1]M_{m:n}(D)E(m,D) \tag{4.8}$$

are independent of K_m, and in fact of the two-component medium altogether.

We have shown that there exist transfer functions relating the initial conditions to the signals at any point in space, and they are seen to have a very special structure. Let us analyze further the properties of these transfer (Green's) functions.

A. Transfer function properties

Let us first analyze the transfer matrices $M_m^n(D)$, for $m<n$. We have by the definition (4.4) that

$$M_m^n(D)=\prod_{i=n-1}^{m}\Theta(i,D)=\begin{bmatrix}[M_m^n(D)]_{11}&[M_m^n(D)]_{12}\\[M_m^n(D)]_{21}&[M_m^n(D)]_{22}\end{bmatrix} \tag{4.9}$$

and from the symmetry and invertibility of the elementary layer transfer functions, we obtain that $M_m^n(D)$ is invertible and obeys

$$\tilde{I}M_m^n(D)\tilde{I} = M_m^n(D^{-1}) \quad \text{with } \tilde{I} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \tag{4.10}$$

Furthermore, the entries of $M_m^n(D)$ are polynomials in D and D^{-1} of degree not more than $n-m$. The determinant of the matrix operator $M_m^n(D)$ is given by the product of the determinants of the $\Theta(i,D)$ appearing in (4.9). We have

$$\det\{\Theta(i,D)\} = F(i)^2/G(i+1)^2[1-K_i^2] \tag{4.11}$$

yielding

$$\det\{M_m^n(D)\} = \prod_{i=m}^{n-1} \frac{F(i)^2}{G(i+1)^2[1-K_i^2]} = \frac{[1-K_{m-1}]G(m)}{[1-K_{n-1}]G(n)}. \tag{4.12}$$

Note that $\det\{M_m^n(D)\}$ approaches 1 as $m \to -\infty$ and $n \to +\infty$, if the potentials approach 1 as the space index increases. Equation (4.12) also shows that the inverse of the transfer matrix from m to n is given by

$$\begin{aligned}[M_m^n(D)]^{-1} &= \frac{[1-K_{n-1}]G(n)}{[1-K_{m-1}]G(m)} \times \begin{bmatrix} [M_m^n(D)]_{22} & -[M_m^n(D)]_{12} \\ -[M_m^n(D)]_{21} & [M_m^n(D)]_{11} \end{bmatrix} \\ &= \frac{[1-K_{n-1}]G(n)}{[1-K_{m-1}]G(m)} \times \begin{bmatrix} [M_m^n(D^{-1})]_{11} & -[M_m^n(D)]_{12} \\ -[M_m^n(D)]_{21} & [M_m^n(D^{-1})]_{22} \end{bmatrix}. \end{aligned} \tag{4.13}$$

Finally, we shall note that the matrices $M_m^n(D)$, when formally regarded as functions of a complex variable $z = D$, obey on the unit circle

$$[M_m^n(e^{j\theta})]\, J\, [M_m^n(e^{j\theta})]^* = \det\{M_m^n(D)\}\, J \tag{4.14}$$

showing that the transfer matrix approaches (as the boundaries tend to $\pm\infty$) a J-unitary matrix (provided it converges, i.e., if its entries have limits as functions of a complex variable z).

The transfer matrices $M_m^n(D)$ yield the wave variables at depth n from those at depth m. It is natural to inquire about the relationship between the waves impinging on a portion of the medium extending from depth m to depth n and the outgoing ones. If the medium is originally at rest, the emerging waves are the causally generated response of the medium layers, since, as we have seen, the scattering descriptions of elementary medium layers are the causal, linear and time-invariant operators (2.13). A few steps of algebra show that the scattering representation corresponding to $M_m^n(D)$ is

$$S_m^n(D) = \frac{1}{[M_m^n(D)]_{22}} \times \begin{bmatrix} \det\{M_m^n(D)\} & [M_m^n(D)]_{12} \\ -[M_m^n(D)]_{21} & 1 \end{bmatrix}. \tag{4.15}$$

Important properties of the scattering representations $S_m^n(D)$ are causality, inherited from the causality of elementary layers the medium is composed of, and asymptotic losslessness due to the J losslessness of the corresponding transfer representation on the unit circle.

We shall see that the data assumed to be available for inverse scattering, a problem that requires the recovery of the local parametrization of a scattering medium described by either a three-term recursion (or partial difference equation) or a two-component evolution equation, are signals that are causally generated in these media. In the case of the wave-propagation description the causality has immediate meaning, however, if we are dealing with the $V(n,D)$ signals, the concept of a causal signal has to be properly defined. We shall show that the Jost solutions as defined in the classical theory of inverse scattering (Case[5]) do indeed correspond to causally generated waves in the equivalent wave propagation media.

B. Causal solutions and inverse scattering

Suppose first that we are dealing with a two-component system corresponding to the discrete Schrödinger equation (1.8), and that we know the medium parametrization up to depth m, i.e., we have $G(m)$ and K_{m-1}. Assume that we are also given an input-response pair $\{W_R(m,D), W_L(m,D)\}$ at $m = 0$, that is right causal, i.e., we know that the $W_{R/L}(n,\tau)$ were zero prior to the time $\tau = 0$ when the first nonzero lag of the sequence $W_R(0,\tau)$ is sent into the medium towards the right. This implies that $W_L(0,\tau)$ will be the causal response elicited by right propagating input signal, and a little thought will show that we have, at depth n,

$$\begin{aligned} &W_R(n,\tau) = 0, \quad \text{for } \tau < n, \\ &W_L(n,\tau) = 0, \quad \text{for } \tau < n+2, \end{aligned} \tag{4.16}$$

simply due to the delay structure of the medium. Also we shall have, immediately (see Bruckstein and Kailath[7]), that

$$W_L(n,\tau = n+2) = K_n W_R(n,\tau = n). \tag{4.17}$$

This observation is the basis of a straightforward inverse scattering process that yields the medium parameters from the data. Indeed, (4.17) readily yields K_0 from the given data, then (2.15) provides $G(1)$, and then we can use (2.16) to determine the sequences $\{W_R(1,D), W_L(1,D)\}$. These sequences are a synthesized set of causal scattering data for the medium starting at depth 2 and extending to $+\infty$, and we can proceed to determine K_1 and $G(2)$, and so on. We thus have an immediate recursive *layer-peeling* procedure that recovers the medium parameters from the scattering data. For more detail on such procedures see Bruckstein and Kailath.[7] We note that the scattering data assumed to be available is equivalent to having the left reflection function of S_0^∞, the scattering representation for the medium portion extending from 0 to $+\infty$. We have, from the structure of the medium, that the nestedness property

$$[S_m^\infty(D)]_{21} = [S_m^n(D)]_{21} + D^{2(n-m)} \times \{\text{a bilinear function of } [S_n^\infty(D)]_{21}\} \tag{4.18}$$

holds, showing that the medium up to depth n can be recovered from the first $2n$ lags of its impulse response alone. There are interesting connections of the above discussed inverse scattering method to an algorithm by Schur for testing for boundedness inside the unit circle, analytic functions of a complex variable (see Schur,[2] Kailath,[6] and Bruckstein and Kailath[7]).

Suppose now that we are dealing with scattering associated to the original three-term recursion (1.8), and assume that the potential sequence $G(n)$ is different from 1 only somewhere between $n=0$ and $n=N>0$. In this case we know that solutions of (1.8) in the "outer" regions $(-\infty,0]$ and $[N,+\infty)$, are of the form $\phi_R(0,D)D^n+\phi_L(0,D)D^{-n}$ and $\phi_R(N,D)D^n+\phi_L(N,D)D^{-n}$, respectively. Only two of the four $\phi_{R/L}(0/N,D)$ functions are independent, and those may be determined if we are given the signals $V(\cdot,D)$ at any two points in space. If we consider the Jost-type solution (see Case[5]), for which $V^J(n,D)=D^n$ for $n>N$, then it is easy to see from the influence propagation diagrams (Fig. 3) that we have for all n that

$$V^J(n,D)=\sum_{i=n}^{\infty} D^i\Omega(n,i)\,. \tag{4.19}$$

Since by definition the sequences $V^J(n,D)$ obey the recursion (1.8), we readily obtain that the potential can be computed from the function $\Omega(\cdot,\cdot)$ as

$$G(n)=\Omega(n-1,n-1)/\Omega(n,n)\,, \tag{4.20}$$

therefore, an inversion algorithm could be based on first determining the kernels $\Omega(\cdot,\cdot)$. The classical approach to inverse problems was to derive integral/matrix equations relating the kernels $\Omega(n,i)$ to the scattering (or so-called spectral) data, and then using (4.20) to recover the potentials. We shall outline here an alternative approach, which exploits the structure of the problem directly, and recovers the potentials by propagating a nonlinear difference equation. The insight that yields immediate derivations of these results follows from the equivalent two-component evolution equations that can always be associated to three-term Schrödinger recursions.

The scattering data that we shall assume available are the functions $\phi^J_{R/L}(D)$ that specify the behavior of $V^J(n,D)$ in the region $(-\infty,0]$. First let us see what is the meaning of a Jost-type solution in the equivalent wave propagation representation. We have at depth $n>N$, that $V(n,D)=D^n$ and also that $V(n+1,D)=D^{n+1}$, and using (4.6) we obtain

$$\begin{aligned} W_R(n,D)&=D^n\{1-[1+K_n]D^2\}\\ &\quad\times\{1+D^2+D^4+D^6+\cdots\}\,, \\ W_L(n,D)&=D^{n+2}K_n\{1+D^2+D^4+D^6+\cdots\}\,, \end{aligned} \tag{4.21}$$

where K_n is the local reflection coefficient at depth n in some equivalent two-component model, and the formal expansion $1/(1-D^2)=1+D^2+D^4+D^6+\cdots$ was also used. An interesting fact becomes clear from this exercise: the waves corresponding to the Jost solutions are *causal* pairs in the region $n>N$. Let us look at what happens at the other edge of the medium, at $n=0$. Assuming without loss of generality that $G(0)=1$, we have that $V^J(0,D)=\phi_R(D)+\phi_L(D)$ and $V^J(-1,D)=\phi_R(D)D^{-1}+\phi_L(D)D$. Using (4.6) again we obtain the following expressions for the waves:

$$\begin{aligned} W_R(0,D)&=1/(1-K_{-1})\{\phi_R(D)[[1-K_{-1}]-D^2]\\ &\quad-\phi_L(D)K_{-1}\}\{1+D^2+D^4+D^6+\cdots\}, \\ W_L(0,D)&=1/(1-K_{-1})\{\phi_R(D)D^2K_{-1}\\ &\quad+\phi_L(D)[1-[1-K_{-1}]D^2]\}\\ &\quad\times\{1+D^2+D^4+D^6+\cdots\}\,. \end{aligned} \tag{4.22}$$

It can be seen that, provided $\phi_L(D)$ has a D^2 factor and is causal, the waves at $n=0$ will constitute a causal pair of scattering data. It is relatively easy to show, using the structure of the wave-propagation medium that we shall have a causal pair at all depth n. This follows from the relation (4.3) and the form of $[M_n^m(D)]^{-1}$.

Therefore the Jost solutions are causal, in the sense of corresponding to causal waves for any choice of equivalent reflection coefficient sequence. The straightforward layer-peeling algorithm can now be invoked to recover the potential over the region $[0,N]$. If we would have chosen $K_{-1}=0$, and assuming that this choice yields a legal two-component model, we would have that

$$W_R(1,D)=\phi_R(D)\quad\text{and}\quad W_L(1,D)=\phi_L(D) \tag{4.23}$$

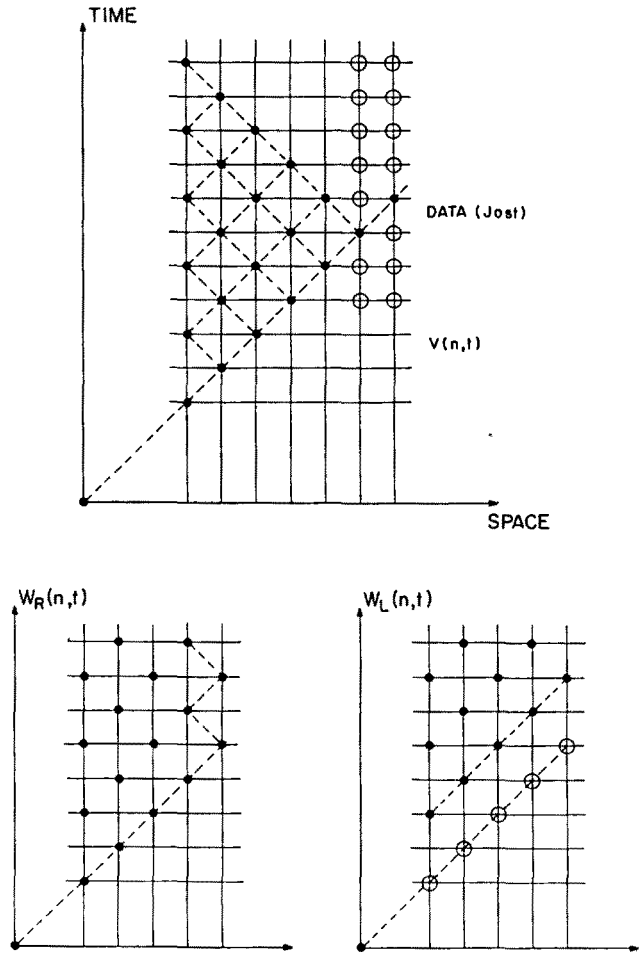

FIG. 3. Causality of Jost solutions.

and we could start propagating the layer-peeling algorithm on this data. Note that we can never recover both $F(n)$ and $G(n)$ in the general equation (1.9) since the recovery of the local reflection coefficient sequence provides recursions for a nonlinear combination of these parameters. Therefore we can use this method to recover the parameters of either the classical discrete Schrödinger equation (1.8), or of a variant for which only $F(n)$ are different from 1, and there exists a mapping between such equations based on a renormalization, see, e.g., Case.[8] Also it is important to note that if we assumed $K_{-1}=0$ and the algorithm yields a $K_{n_c}=1$ at some point, we can continue the medium recovery from this point on by recomputing the scattering data under the assumption of another K_n. This can be done by obtaining $V(n_c-1,D)$ and $V(n_c-2,D)$, say, and recomputing via (4.5) the waves with a different K_{n_c-1}.

It is clear that if we are given the Jost functions, we can obtain alternative causal pairs by assuming that the behavior in the region $n>N$ is $V^C(n,D)=D^n$ (*a causal function*), since this corresponds to convolving the input and output waves at $n=0$ with the same causal function. Sometimes the scattering data is given by an equivalent set of functions, for which, at $n<0$ we have

$$V^C(n,D)=D^n+s(D)D^{-n}=V^J(n,D)/\phi_L(0,D)\,. \tag{4.24}$$

Here $s(D)=[\phi_L(0,D)]/[\phi_R(0,D)]$ and we consider its causal expansion, starting with D^2, a property inherited from $\phi_L(0,D)$. The pair $W_R(0,D)=1$ and $W_L(0,D)=s(D)$ form a causal impulse response pair for the scattering medium associated with the Schrödinger equation, having $K_{-1}=0$ as the "anchor" reflection coefficient and we shall be able to recover the sequence $G(n)$ from this data, via layer peeling.

In his paper on one-dimensional inverse scattering Case[5] tests an inversion method, based on the discrete version of the classical theory that proceeds via Gel'fand–Levitan or Marchenko systems of equations, on an example that corresponds to the following one. Assume $s(D)$ of (4.24) is given as

$$\begin{aligned} s(D)&=D^2\left\{\frac{D^2-1}{(2-g)D^2-g}-1\right\}\\ &=\left(\frac{1}{g}-1\right)D^2+\left(\frac{2-g}{g^2}-\frac{1}{g}\right)D^4\\ &\quad+\left(\frac{(2-g)^2}{g^3}-\frac{2-g}{g^2}\right)D^6+\cdots\,. \end{aligned} \tag{4.25}$$

Applying the layer-peeling inversion algorithm on the pair of sequences $\{1,s(D)\}$ is seen to yield

$$\begin{aligned} &K_0=\frac{1}{g}-1\,,\quad K_1=\frac{(1-g)}{-(1-g)+\frac{1}{2}}\,,\\ &K_2=\frac{(1-g)}{-2(1-g)+\frac{1}{2}}\,, \end{aligned} \tag{4.26}$$

which provide, via (2.17) and assuming $G(n)=1$ for $n\leqslant 0$, the potential sequence

$$G(1)=g,\quad G(2)=1,\quad G(3)=1, \tag{4.27}$$

a result that coincides, up to a shift in space, with that obtained by Case.[5]

V. CONCLUDING REMARKS ON BOUND STATES

We have presented a rather direct approach to the analysis of three-term recursions by mapping them into two-component wave-propagation equations having a certain delay-and-interaction structure. Note that we have assumed that the propagating signals are general time sequences and used their representation as formal power series, or generating functions. This immediately puts us into the domain of so-called scattering solutions of Schrödinger equations, therefore we did not discuss issues pertaining to the existence of so-called bound states. Indeed note that once Eqs. (1.8) or (1.9) is written as an eigenvalue problem

$$\begin{aligned} &F(n+1)V(n+1,\lambda)+F(n)V(n-1,\lambda)\\ &\quad=G(n)2\lambda V(n,\lambda)\,, \end{aligned} \tag{5.1}$$

it receives more mathematical content than that implied by its interpretation as a wave-propagation equation. The spectrum of values for λ where solutions exist consists of the values $\lambda=\cos\theta\in[-1,1]$, for which $D=e^{j\theta}$, and can have the interpretation of a delay operator in the harmonic analysis of time sequences, but we may also ask what happens for values of λ outside the itnerval $[-1,1]$. If a solution to (5.1) exists for such a value of λ, then we shall have that $D\in\mathbf{R}$, i.e., it will be a real value, since

$$D+D^{-1}=2\lambda \tag{5.2}$$

implies that

$$D_{1,2}=\lambda\pm[\lambda^2-1]^{1/2}\,,$$

which also shows, incidentally, that $D_1=D_2^{-1}$.

In our two-component interpretation, the waves then disappear in a rather mysterious way and are replaced by single values at each point in space (or rather, time sequences will be have a constant value at all times). The D operators become pure gains, instead of delays, and the solutions of (5.1) effectively become sequences in only the space dimension. If we want these sequences to be bounded and have finite energy, it turns out that there is only a discrete spectrum of values of λ for which such solutions exist. Suppose that we have a medium described by a sequence of potentials for which the reflection coefficients are very close to zero outside an interval $[0,N]$. Then we have that $M_0^N(D)$ describes the interaction of signals that exist at $n=0$ and those at $n=N$. In order to have bounded solutions corresponding to some real value $D=d_i<1$, we need to have, see Fig. 4,

$$W_R(N,d_i)\neq 0\quad\text{and}\quad W_L(0,d_i)\neq 0 \tag{5.3a}$$

together with

$$W_R(0,d_i)=0\quad\text{and}\quad W_L(N,d_i)=0 \tag{5.3b}$$

proving that in this case we shall have $[M_0^N(d_i)]_{22}=0$. Therefore, to have a bound-state solution, $[M_0^N(D)]_{22}$ has to have zeros inside the unit circle. The alternative analysis of $d_j>1$ leads to the same conclusion, viz. $[M_0^N(D)]_{11}$ needs to have zeros outside the unit circle. This condition however implies that the scattering matrix (4.15) has poles

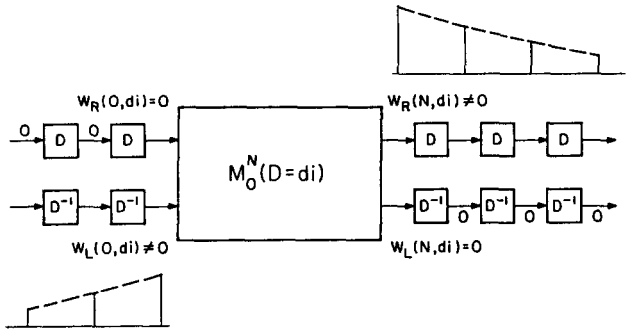

FIG. 4. Conditions for the existence of bound states.

inside the unit circle, which means that, from a system theoretical point of view, the wave-scattering system is unstable, i.e., some inputs will elicit exponentially growing causal responses. This did not bother us much, since all along we were not concerned with the boundedness of our functions, or with the convergence of the generating functions to legal and analytic functions in the complex variable D. We, however, obtained sufficient conditions under which such problems do not arise: indeed it is easy to realize that if the medium can be associated to a lossless structure we shall never have bound state solutions. Also if we stay in the scattering domain and deal with sequences represented by purely formal generating functions, we can apply the straightforward analysis without any problems. If we want to deal with sequences of numbers that are bounded and summable in some sense, we should only use inputs that do not excite the unstable modes of the scattering medium. These issues underlie much of the effort in the rigorous treatment of discrete inverse scattering problems, however, we feel that the simplicity of the approach outlined in this paper explains the mechanism of inverse scattering in a way that most directly exploits the wave interaction model assumed.

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Time-dependent canonical formalism of thermally dissipative fields and renormalization scheme

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The canonical formalism of thermally dissipative semifree fields in the time-dependent situation is presented. The use of thermal covariant derivatives simplifies the formulation considerably. With this formalism one can unambiguously obtain the interaction Hamiltonian under any thermal situation which together with the free propagator enables perturbative calculations to be performed. The "on-shell" renormalization condition in the time-dependent case is also discussed. The model of a system with a thermal reservoir illustrates how the present formalism works in time-dependent situations.

I. INTRODUCTION

Thermo field dynamics (TFD) is a real time quantum field theory with thermal degrees of freedom. In a series of papers[1-7] we have been extending TFD to describe any thermal situation, including nonequilibrium phenomena. This extended TFD has been shown to be equivalent to the density matrix formalism with the Liouville equation.[1] The purpose of this paper is to present this extended TFD in a systematic form placing a strong emphasis on the time dependence of thermal situations.

Before starting on the extended TFD we summarize here the equilibrium TFD[8,9] that is now well established. The basic concepts in equilibrium TFD are the following: (i) the doubling of each degree of freedom through the *tilde conjugation rules*, (ii) the thermal Bogoliubov transformation taking care of the freedom in choice of the temperature, and (iii) the total Lagrangian density is given by

$$\hat{\mathscr{L}} = \mathscr{L} - \tilde{\mathscr{L}}, \tag{1.1}$$

where $\mathscr{L}$ is the usual Lagrangian density and $\tilde{\mathscr{L}}$ is obtained from $\mathscr{L}$ by the tilde conjugation rules.

According to (i), with an operator A we associate with it its tilde conjugate $\tilde{A}$. The tilde-conjugation rules are summarized in the next section. In TFD, therefore, any field has its tilde conjugate, forming a thermal doublet. A similar situation of the doubling of the degrees of freedom is observed in other formulations of real-time quantum field theory at finite temperature such as the C^*-algebraic formalism,[10] the path-ordering formalism of the Schwinger–Keldysh type,[11] and the superoperator formalism[12] of the Liouville equation. The relation between TFD and the C^*-algebraic formalism was beautifully analyzed by Ojima in Ref. 13. The relation between TFD and the path-ordering method was clarified in Ref. 14. In the theory of the density matrix there appear right- and left-operating operators which form thermal doublets and which are called the superoperators.[12] The relationship between the superoperator formalism and TFD was given in Ref. 1. Intuitively speaking, the nontilde operators take care of the usual quantum excitations, while the tilde operators describe the thermal excitations.[8]

Since each field is a thermal doublet, there appears a mixing of the doublet components through the Bogoliubov transformations. In the equilibrium TFD the different choices of temperature correspond to different choices of these Bogoliubov transformations. Thus we were led to the concept (ii), i.e., the thermal Bogoliubov transformation.

The concept (iii) for the total Lagrangian in TFD exhibits the following beautiful feature of TFD. Since $\mathscr{L}$ does not depend on the temperature, neither does $\hat{\mathscr{L}}$. The temperature appears only through the thermal Bogoliubov transformations. Since these features play a fundamental role in the extension of TFD to nonequilibrium situations let us elaborate on them. As is well known the language of quantum field theory has a dual structure.[8] The basic entities such as the Lagrangian, the Heisenberg equations, and the basic canonical commutation relations are expressed in terms of the basic fields called the Heisenberg operators, while the phenomenological language is constructed in terms of the "quasiparticle" operators, which are the particles *including all the renormalization effects*. The state-vector space is the Fock space associated with these quasiparticles. When a Lagrangian is given, an essential task in quantum field theory is to obtain the expressions for the Heisenberg operators written in terms of the quasiparticle operators. This expression, which has been frequently called the dynamical map,[8] determines the realization of the Heisenberg operators. The different choices of the thermal Bogoliubov transformation correspond to different choices of the realization of the Heisenberg operators. Thus concepts (i) and (ii) imply that different temperatures correspond to the different realization of the Heisenberg operators that are determined by the total Lagrangian $\hat{\mathscr{L}}$. Since the state-vector space is the Fock space associated with the quasiparticles, the best choice for the unperturbed Hamiltonian is the Hamiltonian of the quasiparticles. Denoting the annihilation and creation operators by $(\xi_k, \tilde{\xi}_k)$ and $(\xi_k^\dagger, \tilde{\xi}_k^\dagger)$, respectively (i.e., $\xi_k|0\rangle = \tilde{\xi}_k|0\rangle = 0$ and $\langle 0|\xi_k^\dagger = \langle 0|\tilde{\xi}_k^\dagger = 0$ with the thermal vacua $|0\rangle$ and $\langle 0|$, where k represents any quantum number), the Fock space is constructed by the cyclic operation of creation operators on $|0\rangle$ and of annihilation operators on $\langle 0|$. Denoting the quasiparticle energy by ω_k, the temporal behavior of the creation and annihilation operators

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are required to be of the form

$$\xi_k(t) = \xi_k E_k(t), \quad \tilde{\xi}_k(t) = \tilde{\xi}_k E_k^*(t) \tag{1.2}$$

with $E_k(t) = \exp(-i\omega_k t)$. Then, the feature (ii) means that the oscillator operators $(a_k(t), \tilde{a}_k(t))$ of the fields are related to $(\xi_k(t), \tilde{\xi}_k(t))$ through the Bogoliubov transformation B,

$$\begin{bmatrix} a_k(t) \\ \tilde{a}_k^\dagger(t) \end{bmatrix} = B \begin{bmatrix} \xi_k(t) \\ \tilde{\xi}_k^\dagger(t) \end{bmatrix}, \tag{1.3}$$

where B is a 2×2 matrix.

A remarkable fact in equilibrium TFD is that the loop corrections to the self-energy of the quasiparticles create an imaginary term, making the quasiparticles dissipative (spontaneous creation of dissipation). This dissipative behavior is caused by the presence of the background tilde field whose quanta carry negative energy. The real quanta described by the nontilde operators live in a world with the background tilde field of negative energy, which easily absorbs the energy of real quanta and makes them dissipative. An essential reason why the quasiparticles easily become dissipative, irrespective of the fact that the Lagrangian $\hat{\mathscr{L}}$ is real, is that the quantum field has an infinite number of degrees of freedom. When we denote the number of degrees of freedom by N, the $(1/N)$ expansion provides us with a clear picture for the spontaneous creation of dissipation. The leading term in the $(1/N)$ expansion exhibits the dissipative behavior. Since the Lagrangian is real when N is finite the dissipative behavior disappears when all of the terms in the $(1/N)$ expansion are summed up. However, when N is infinite and only the leading term in the expansion is picked up, the dissipative behavior may arise from a real Lagrangian. This consideration will be explicitly demonstrated in the analysis of the reservoir model in Sec. V. The appearance of a dissipative effect in the equilibrium situation is not surprising. Although the equilibrium situation is stationary, a short-time measurement induces excited states which approach the ground state dissipatively. Thus although the thermal average of the observable is independent of time, the dissipative effect appears in the multipoint functions such as Green's functions and correlation functions.

The same dissipative effect becomes apparent even in the thermal average of observables when the thermal situation becomes nonstationary. Even a brief consideration[2] of a time-dependent transition between a disordered state and an ordered state indicates that the renormalization effects due to loop corrections become dependent on time, making most of the physical quantities (such as energy, order parameter, dissipative coefficient, particle number, etc.) dependent on time. This analysis also indicated a need for time-dependent renormalization.[2] This motivates us to extend TFD to time-dependent nonequilibrium phenomena.

The task of extending TFD began with the construction of the Hamiltonian for dissipative quasiparticle.[1,2,4] The idea is that once this Hamiltonian, say $\hat{H}^0$, becomes known the interaction Hamiltonian is given by $\hat{H} - \hat{H}^0$, where $\hat{H}$ is the Hamiltonian obtained from the total Lagrangian $\hat{\mathscr{L}}$. This provides us with the Feynman-diagram method for computation. In the density matrix formalism the description of an open system in terms of quasiparticles was obtained by eliminating the variables of the reservoir through the coarse graining process. Our first approach[1] was to reformulate this coarse graining process in terms of the TFD formalism. In Ref. 3 this approach was reformulated in terms of the Green's function formalism and the result was compared with the path-ordering method. Our next step, made in Ref. 4, was to construct $\hat{H}^0$ by making the so-called thermal state condition time dependent [this is equivalent to making the thermal Bogoliubov transformation (1.3) dependent on time]. It turned out that the $\hat{H}^0$ thus obtained depends on time explicitly. A remarkable fact is that this $\hat{H}^0$ at the long-time limit $(t\to\infty)$ coincides with $\hat{H}^0$ obtained from the coarse graining process. Another significant point in the analysis in Ref. 4 was to point out that the spontaneous creation of dissipation can be formulated in terms of the renormalization technique. The basic idea here is that since the unperturbed quasiparticles include all of the self-energy corrections, and since the self-energy corrections frequently make quasiparticles dissipative, the unperturbed Hamiltonian contains dissipative terms. Thus we are led to the self-consistent renormalization condition which states that the interaction Hamiltonian $(\hat{H} - \hat{H}^0)$ should not create any on-shell self-energy. Since the on-shell self-energy is a 2×2 thermal matrix this condition gives four complex equations, which are equivalent to eight real equations. Although not all of these equations may be independent of each other, this condition does contain more information than the energy ω_k and the dissipative coefficient κ_k. However, the precise formulation of the self-consistent renormalization condition required more analysis and was not presented in Ref. 4. To learn more from this formalism in Ref. 4 we applied it to two models in the stationary case in Ref. 5, one of which was an exactly solvable reservoir model. Since TFD treats the reservoir as a part of the quantum field system we do not need to eliminate the reservoir variables. This analysis clearly exhibits the previously mentioned argument based on the $(1/N)$ expansion with the limit $N\to\infty$. The other model was a real scalar field model without a reservoir. Since, as was pointed out above, TFD treats a reservoir as a part of a quantum field system, it is readily applicable to any quantum field system without any reservoir. Here it is important to note that a quantum field has an infinite number of degrees of freedom as the reservoir does and also that a stochastic effect is caused by the background tilde field, which has negative energy. In any application of the formalism to a quantum field system it is important to put the theory of dissipative quasiparticle in the canonical form. This was done in Ref. 6. However, this just dealt with the stationary case.

With all of the results mentioned above, we are now ready to put the foundations of nonequilibrium TFD in a systematic form. This is the purpose of this paper. The exactly solvable reservoir model in a time-dependent situation will be treated as an example. The foundations of nonequilibrium TFD are the previously-mentioned basic concepts, (i), (ii), and (iii). We now state that any (even time-dependent) Bogoliubov transformation, which is consistent with other basic concepts, is permitted and that *the entire set of the Bogoliubov transformations cover all possible thermal phe-*

nomena. In other words, the general TFD considers all possible realizations of the Heisenberg fields controlled by the Lagrangian $\hat{\mathscr{L}}$. In the equilibrium TFD we considered only a particular set of Bogoliubov transformations. To cover the time-dependent phenomena, we consider time-dependent Bogoliubov transformation. Furthermore, since the quasiparticle is dissipative we might assume that $E_k(t)$ in (1.2) is $\exp(-i\omega_k t-\kappa_k t)$ with unknown parameters ω_k and κ_k. However, we find that when a time-dependent thermal situation is considered the higher-order loop corrections may make ω_k and κ_k dependent on time. *We thus state that the dissipative quasiparticles are defined by* $(\xi_k(t),\xi_k^\dagger(t))$ *with*

$$E_k(t)=\exp\left[\int_0^t ds\{-i\omega_k(s)-\kappa_k(s)\}\right].$$

This dissipative quasiparticle is called the "semifree" quasiparticle. The appearance of κ_k in $E_k(t)$ and the time-dependent Bogoliubov transformation are the basic features in the extended TFD. Our unperturbed particles are the fully renormalized semifree quasiparticles. Since these particles are fully renormalized the interaction Hamiltonian (which contains the renormalization counter terms) should not create any on-shell correction. This leads to the self-consistent renormalization condition which, in general, depends on time.

The extended TFD distinguishes itself from the equilibrium one by the fact that the unperturbed Hamiltonian $\hat{H}^0$ is not the usual free Hamiltonian, but the semifree Hamiltonian which has an imaginary term responsible for the dissipative effects. Then we need the full knowledge of the semifree field in order to perform a perturbative calculation formulated in the terminology of the interaction representation. We first formulate the extended TFD in terms of the oscillator operators $a(\mathbf{k})$ and $a^\dagger(\mathbf{k})$. It is not an easy task to formulate the extended TFD in terms of field operators $\psi(x)$ and $\bar{\psi}(x)$ when the formalism is required to include any time-dependent thermal situation. In order to construct such a formalism one requires a method simpler and more systematic than those that have previously been presented. In this paper the formulation of the extended TFD begins with the time-dependent Bogoliubov transformation applied to a semifree field. This leads us to the thermal covariant derivatives that simplify the construction of the extended TFD.

The reconstruction of the generalized semifree oscillator operators[4] is given in Sec. II by use of the thermal covariant derivatives. Then by using the same method we formulate a theory of semifree fields which is applicable to time-dependent thermal phenomena. Although the use of the time-dependent Bogoliubov transformation and the covariant derivatives simplified the formulation of semifree fields, the consideration in Sec. III is still limited to semifree fields of type 1 (i.e., the semifree fields with a positive frequency part only). Study of semifree fields of type 2 (i.e., those with both the positive and negative frequency parts) is limited to time-independent situations only. This is presented in the Appendix. The works in the past[4,7] showed that there exists a flexibility in the formulation of TFD: TFD carries an arbitrary parameter denoted by α. In equilibrium TFD it has been shown[14] that the freedom in choice of α corresponds to the freedom in choice of path in the path-ordering method. This might lead us to anticipate that this freedom might disappear in nonequilibrium TFD. Contrary to this expectation, *this freedom remains in nonequilibrium* TFD. This means that the choice of α is not intrinsically related to the choice of path in the path-ordering method. Furthermore, the consideration in Sec. II will show that the formulation of TFD has a wider choice of arbitrary parameters. The entire consideration in this paper is made without specifying these parameters.

Once we have a formulation of the semifree field we try to develop the perturbative calculation in the extended TFD including the time-dependent situation by using a semifree quasiparticle field for the unperturbed field. To do this we need the knowledge of the interaction Hamiltonian. A method for identifying the interaction Hamiltonian is presented in Sec. IV. The argument there begins with the fact that the TFD Lagrangian density is given by $\hat{\mathscr{L}}=\mathscr{L}-\bar{\mathscr{L}}$ and the Hamiltonian $\hat{H}$ in TFD follows from $\hat{\mathscr{L}}$ through the usual route in the canonical theory. The Hamiltonian $\hat{H}^0$ of the semifree quasiparticle field is given in Sec. III. Then the interaction Hamiltonian in the extended TFD is found to be $\hat{H}_{\rm int}=\hat{H}-\hat{H}^0$.

In the perturbative calculation in the extended TFD a vital step is the renormalization procedure which leads to a set of so-called *self-consistent equations*.[4,5] The latter equations determine not only the renormalized energy and the dissipative coefficient, but also the temporal behavior of the average number density when the initial value of the average number density is given. Any renormalization procedure is based on the on-shell renormalization condition which is associated with the renormalization point. In previous papers the on-shell renormalization condition has been given only for the time-independent case, so in Sec. V *we formulate the on-shell renormalization condition for time-dependent thermal situations*. This renormalization method is applied to a simple solvable model to illustrate how the energy and dissipative coefficients as well as temporal behavior of the average number density can be determined. We find a nonvanishing dissipative coefficient (spontaneous creation of dissipation).

Section VI is devoted to a brief description of the physical mechanism for the appearance of the dissipative coefficient in an isolated quantum field system. There, the importance of the infinite degrees of freedom and the presence of the negative energy background field (tilde quanta) is explained in terms of the $(1/N)$-power expansion method. A similarity between the mechanism of spontaneous breakdown of symmetries and the one for spontaneous creation of dissipation is also pointed out. A discussion on the relation between the spontaneous creation of dissipation and the spontaneous breakdown of time-translation symmetry is also presented. It will be pointed out what kinds of problems still remain in order to complete the extended TFD.

II. RECONSTRUCTION OF THE GENERAL SEMIFREE HAMILTONIAN IN TFD

We start by introducing certain quasiparticle annihilation and creation operator $\xi(\mathbf{k})$ and $\xi^\dagger(\mathbf{k})$ in the interaction

representation with the thermal vacua $|0\rangle$, $\langle 0|$:

$$\xi(\mathbf{k})|0\rangle = 0, \tag{2.1a}$$

$$\langle 0|\xi^{\dagger}(\mathbf{k}) = 0. \tag{2.1b}$$

These operators obey the commutation relation

$$[\xi(\mathbf{k}),\xi^{\dagger}(\mathbf{l})]_{\sigma} = \delta(\mathbf{k}-\mathbf{l}), \tag{2.2}$$

where the σ commutator is defined by

$$[A,B]_{\sigma} = AB - \sigma BA, \tag{2.3}$$

with $\sigma = 1$ for boson operators and $\sigma = -1$ for fermion operators. The other commutators vanish. We suppressed all indices representing spin and any other internal degrees of freedom other than the momentum $\mathbf{k}$. For simplicity we will drop the momentum variable in the section below unless it is required.

It is now widely known that in TFD with an operator A we associate with it its tilde conjugate $\tilde{A}$ according to the rules

$$(AB)^{\sim} = \tilde{A}\tilde{B}, \tag{2.4a}$$

$$(c_1A + c_2B)^{\sim} = c_1^{*}\tilde{A} + c_2^{*}\tilde{B} \quad (c_1,c_2 \text{ are } c \text{ numbers}), \tag{2.4b}$$

$$(A^{\dagger})^{\sim} = \tilde{A}^{\dagger}, \tag{2.4c}$$

$$(\tilde{A})^{\sim} = \sigma A, \tag{2.4d}$$

$$|0\rangle^{\sim} = |0\rangle, \quad \langle 0|^{\sim} = \langle 0|. \tag{2.4e}$$

Taking the tilde conjugate of (2.1) and (2.2) we get

$$\tilde{\xi}|0\rangle = 0, \tag{2.5a}$$

$$\langle 0|\tilde{\xi}^{\dagger} = 0, \tag{2.5b}$$

$$[\tilde{\xi}(\mathbf{k}),\tilde{\xi}^{\dagger}(\mathbf{l})]_{\sigma} = \delta(\mathbf{k}-\mathbf{l}). \tag{2.6}$$

The σ-commutation relations between tilde and nontilde operators are assumed to vanish. Equations (2.1) and (2.5) are called the thermal state conditions.

For later convenience we introduce the thermal doublet notation

$$\xi^{\mu} = \begin{bmatrix} \xi \\ \tilde{\xi}^{\dagger} \end{bmatrix}^{\mu}, \quad \bar{\xi}^{\mu} = [\xi^{\dagger} - \sigma\tilde{\xi}]^{\mu} \quad (\mu = 1,2). \tag{2.7}$$

Then we write (2.2) and (2.6) compactly as

$$[\xi^{\mu},\bar{\xi}^{\nu}]_{\sigma} = \delta^{\mu\nu}. \tag{2.8}$$

We now introduce $\xi(t)^{\mu}$ and $\bar{\xi}(t)^{\mu}$ with the form

$$\xi(t)^{\mu} = E_0(t)^{\mu\nu}\xi^{\nu}, \tag{2.9a}$$

$$\bar{\xi}(t)^{\mu} = \bar{\xi}^{\nu}E_0^{-1}(t)^{\nu\mu}, \tag{2.9b}$$

where

$$E_0(t) = \exp\left[-i\int_0^t ds\{\omega(s) - i\kappa_0(s)\tau_3\}\right]. \tag{2.10}$$

We call $\xi(t)^{\mu}$ and $\bar{\xi}(t)^{\mu}$ the semifree quasiparticle operators.

Our state vector space, called the thermal space, is the linear space spanned by the set of bra and ket state vectors that are generated by cyclic operations of the annihilation operators ξ^1 and $\bar{\xi}^2$ on the thermal vacuum $\langle 0|$, and of the creation operators ξ^2 and $\bar{\xi}^1$ on $|0\rangle$.

Let us now identify how the quasiparticle creation and annihilation operators are related to the variables describing a quantum field system. A usual choice for variables is harmonic oscillator-type operators, a and $a^{\dagger}$, satisfying $[a(\mathbf{k}),a^{\dagger}(\mathbf{l})]_{\sigma} = \delta(\mathbf{k}-\mathbf{l})$. In TFD these operators also form thermal doublets. Introducing the notations

$$a(t) = \hat{S}_a^{-1}(t)a\hat{S}_a(t), \tag{2.11a}$$

$$a^{\dagger\dagger}(t) = \hat{S}_a^{-1}(t)a^{\dagger}\hat{S}_a(t), \tag{2.11b}$$

where the time-translation operator $\hat{S}_a(t)$ will be specified later, the thermal doublets are

$$a(t)^{\mu} = \begin{bmatrix} a(t) \\ \tilde{a}^{\dagger\dagger}(t) \end{bmatrix}^{\mu}, \quad \bar{a}(t)^{\mu} = [a^{\dagger\dagger}(t) - \sigma\tilde{a}(t)]^{\mu}. \tag{2.12}$$

The thermal state conditions for $a(t)^{\mu}$ and $\bar{a}(t)^{\mu}$ in TFD (cf. Ref. 4) can be rephrased by the statement that these operators in the interaction representation are related to $\xi(t)^{\mu}$ and $\bar{\xi}(t)^{\mu}$ through a generalized Bogoliubov transformation

$$a(t)^{\mu} = b^{-1}(t)^{\mu\nu}\xi(t)^{\nu}, \tag{2.13a}$$

$$\bar{a}(t)^{\mu} = \bar{\xi}(t)^{\nu}b(t)^{\nu\mu}. \tag{2.13b}$$

In this paper we use these as basic relations in TFD, rather than the thermal state conditions for a and $\bar{a}$. The above relations give the commutation relation

$$[a(t)^{\mu},\bar{a}(t)^{\nu}] = \delta^{\mu\nu}. \tag{2.14}$$

For the consistency of the tilde conjugation rules (2.4) for both a and ξ, we must have

$$\det b(t) = 1. \tag{2.15}$$

The observable average number density $n(t)$ is given in terms of $a(t)$ and $a^{\dagger\dagger}(t)$ by

$$n(t) = \langle 0|a^{\dagger\dagger}(t)a(t)|0\rangle. \tag{2.16}$$

Let us express the matrix b by

$$b(t) = \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix}. \tag{2.17}$$

Using (2.13) together with (2.9) and considering the definitions of the quasiparticle creation and annihilation operators, (2.1), (2.2), (2.5), and (2.6), together with the unimodular nature of b, (2.15), we find that

$$b_{12}b_{21} = \sigma n(t), \tag{2.18a}$$

$$b_{11}b_{22} = 1 + \sigma n(t). \tag{2.18b}$$

From (2.18) it follows that the matrix $b(t)$ contains two free parameters. We can therefore write $b(t)$ as

$$b(t) = W_L^{-1}(t)B_0(t)W_R(t), \tag{2.19}$$

where

$$B_0(t) = \begin{bmatrix} 1+\sigma n(t) & -\sigma n(t) \\ -1 & 1 \end{bmatrix}, \tag{2.20a}$$

$$W_L(t) = \exp[\tau_3 \ln b_L(t)], \tag{2.20b}$$

$$W_R(t) = \exp[\tau_3 \ln b_R(t)]. \tag{2.20c}$$

The two arbitrary parameter b_L and b_R, which generally depend on time and momentum, etc., are related to b_{21} and b_{22} by

$$b_L^2 = -b_{21}b_{22}, \tag{2.21a}$$

$$b_R^2 = -b_{21}/b_{22}. \tag{2.21b}$$

The parameter b_R is related to the thermal state condi-

tions (2.1) and (2.5), rewritten in terms of $a(t)^{\mu}$ and $\bar{a}(t)^{\mu}$,

$$[a(t)^1 - F(t)a(t)^2]|0\rangle = 0, \tag{2.22a}$$

$$[\bar{a}(t)^2 + F(t)a(t)^1]|0\rangle = 0, \tag{2.22b}$$

$$\langle 0|[\bar{a}(t)^1 + \sigma f(t)F^{-1}(t)\bar{a}(t)^2] = 0, \tag{2.22c}$$

$$\langle 0|[a(t)^2 - \sigma f(t)F^{-1}(t)a(t)^1] = 0, \tag{2.22d}$$

where

$$f(t) = n(t)/[1 + \sigma n(t)], \tag{2.23}$$

$$F(t) = \sigma f(t) b_R^{-2}(t). \tag{2.24}$$

The tilde conjugation of (2.22a) together with (2.21b) shows that $F(t)$, and therefore, $b_R(t)$ should be real. Note that the parameter b_L does not appear in (2.22). In comparison with Refs. 4 and 7 we obtain the previous thermal state conditions if we choose

$$F(t) = f^{\alpha}(t) \tag{2.25}$$

with $0 \leq \alpha \leq 1$. This implies that the arbitrariness of b_R includes the freedom of choice of α in the previous papers.[4,7] However, the present formulation is wider than the previous one since b_R and $F(t)$ are quite arbitrary as far as they are real.

On the other hand, the flexibility of choice of b_L has not been discussed in the previous papers. To take into account this flexibility, we introduce

$$E(t) = W_L(t)E_0(t) \tag{2.26}$$

$$= \exp\left[-i \int_0^t ds\{\omega(s) - i\kappa(s)\tau_3\}\right] \tag{2.27}$$

with

$$\kappa(t) = \kappa_0(t) - \partial_t \ln b_L(t). \tag{2.28}$$

Now (2.13) read as

$$a(t)^{\mu} = B^{-1}(t)^{\mu\rho}E(t)^{\rho\nu}\xi^{\nu}, \tag{2.29a}$$

$$\bar{a}(t)^{\mu} = \bar{\xi}^{\nu}E^{-1}(t)^{\nu\rho}B(t)^{\rho\mu}, \tag{2.29b}$$

with

$$B(t) = B_0(t)W_R(t). \tag{2.30}$$

This motivates us to introduce the *thermal covariant derivatives*,

$$D^{+}(t) = B^{-1}(t)E(t)\partial_t E^{-1}(t)B(t), \tag{2.31a}$$

$$\overleftarrow{D}^{+}(t) = B^{-1}(t)E(t)\overleftarrow{\partial}_t E^{-1}(t)B(t). \tag{2.31b}$$

The equations of motion for $a(t)$ and $\bar{a}(t)$ are

$$iD^{+}(t)^{\mu\nu}a(t)^{\nu} = 0, \tag{2.32a}$$

$$i\bar{a}(t)^{\nu}\overleftarrow{D}^{+}(t)^{\nu\mu} = 0. \tag{2.32b}$$

We obtain from (2.31)

$$D^{+}(t) = \partial_t + i[\omega(t) - iP(t)], \tag{2.33a}$$

$$\overleftarrow{D}^{+}(t) = \overleftarrow{\partial}_t - i[\omega(t) - iP(t)], \tag{2.33b}$$

with

$$P(t) = P_1(t) + P_2(t), \tag{2.34}$$

$$P_1(t) = \kappa(t)A(t) + \sigma\dot{n}(t)\tau(t), \tag{2.35}$$

$$P_2(t) = W_R^{-1}(t)\partial_t W_R(t), \tag{2.36}$$

$$= \partial_t\{\ln b_R(t)\}\tau_3, \tag{2.37}$$

where the various matrices are defined by

$$A(t) = W_R^{-1}(t)A_0(t)W_R(t) = B^{-1}(t)\tau_3 B(t), \tag{2.38}$$

$$A_0(t) = B_0^{-1}(t)\tau_3 B_0(t)$$

$$= \begin{bmatrix} 1 + 2\sigma n(t) & -2\sigma n(t) \\ 2(1 + \sigma n(t)) & -(1 + 2\sigma n(t)) \end{bmatrix}, \tag{2.39}$$

$$\tau(t) = W_R^{-1}(t)\tau_0 W_R(t), \tag{2.40}$$

$$\tau_0 = \begin{bmatrix} 1 & -1 \\ 1 & -1 \end{bmatrix}. \tag{2.41}$$

The equations in (2.32) show that the semifree Hamiltonian for a and $\bar{a}$ is

$$\hat{H}_a^0(t) = \bar{a}(t)^{\mu}[\omega(t) - iP(t)]^{\mu\nu}a(t)^{\nu}. \tag{2.42}$$

This Hamiltonian becomes the one given in Ref. 4 when (2.25) is assumed. It is easy to prove that $\hat{H}_a^0(t)$ is tildian,

$$[i\hat{H}_a^0(t)]^{\sim} = i\hat{H}_a^0(t). \tag{2.43}$$

We have

$$a(t)^{\mu} = \hat{S}_a^{-1}(t)a^{\mu}\hat{S}_a(t), \tag{2.44a}$$

$$\bar{a}(t)^{\mu} = \hat{S}_a^{-1}(t)\bar{a}^{\mu}\hat{S}_a(t), \tag{2.44b}$$

with

$$\partial_t \hat{S}_a(t) = -i\hat{H}_a^0(t)\hat{S}_a(t), \tag{2.45a}$$

$$(\hat{S}_a(t))^{\sim} = \hat{S}_a(t), \tag{2.45b}$$

$$\hat{S}_a(0) = 1. \tag{2.45c}$$

The construction of the semifree Hamiltonian $\hat{H}_a^0(t)$ in this paper is considerably simpler than the one in the previous papers. This is because our consideration in this paper is based on the existence of quasiparticle creation and annihilation operators which form the thermal doublets ξ^{μ} and $\bar{\xi}^{\mu}$, and also on the use of the generalized Bogoliubov transformation. In the next two sections we formulate the semifree field theory, not in terms of oscillator variables $(a,\bar{a})$ but in terms of field variables. There we find the thermal covariant derivatives extremely useful.

III. A GENERAL THEORY FOR SEMIFREE FIELDS

In this section we formulate the semifree field theory in terms of the field variables. Our consideration is confined to fields of type 1 (i.e., fields that contain only the positive frequency part). We have not made the extension to fields of type 2 (i.e., fields which contains both positive and negative frequency parts) in time-dependent situations. In the time-independent case fields of type 2 will be treated in the Appendix.

In this section we consider a Bose field without spin or any other internal degrees of freedom, the extension to general multicomponent fields being straightforward.

We consider thermal doublet semifree fields, say $\psi(x)^{\mu}$ and $\bar{\psi}(x)^{\mu}$, which are linear in the semifree operators $a(t,\mathbf{k})^{\mu}$ and $\bar{a}(t,\mathbf{k})^{\mu}$, considered in the last section. Following the assumption in the usual quantum field theory we require that the time development of ψ and $\bar{\psi}$ is controlled by the operator $\hat{S}_a(t)$ in (2.44),

$$\psi(x)^{\mu} = \hat{S}_a^{-1}(t)\psi(t = 0,\mathbf{x})^{\mu}\hat{S}_a(t), \tag{3.1a}$$

$$\bar{\psi}(x)^{\mu} = \hat{S}_a^{-1}(t)\bar{\psi}(t = 0,\mathbf{x})^{\mu}\hat{S}_a(t), \tag{3.1b}$$

where x stands for $(t,\mathbf{x})$. Therefore we expand $\psi(x)$ and $\bar{\psi}(x)$ as

$$\psi(x)^{\mu} = \int d^3k\, U(\mathbf{x},\mathbf{k})^{\mu\nu} a(t,\mathbf{k})^{\nu}, \tag{3.2}$$

$$= \int d^3k\, u(x,\mathbf{k})^{\mu\nu} a(\mathbf{k})^{\nu}, \tag{3.3}$$

$$\bar{\psi}(x)^{\mu} = \int d^3k\, \bar{a}(t,\mathbf{k})^{\nu} \overline{U}(\mathbf{x},\mathbf{k})^{\nu\mu}, \tag{3.2'}$$

$$= \int d^3k\, \bar{a}(\mathbf{k})^{\nu} \bar{u}(x,\mathbf{k})^{\nu\mu}, \tag{3.3'}$$

where U, $\overline{U}$, u, and $\bar{u}$ are certain c number 2×2 matrix wave functions. According to (2.29), u and $\bar{u}$ are related to U and $\overline{U}$, respectively, in the following way:

$$u(x,\mathbf{k}) = U(\mathbf{x},\mathbf{k}) B^{-1}(t,\mathbf{k}) E(t,\mathbf{k}) B(0,\mathbf{k}), \tag{3.4a}$$

$$\bar{u}(x,\mathbf{k}) = B^{-1}(0,\mathbf{k}) E^{-1}(t,\mathbf{k}) B(t,\mathbf{k}) \overline{U}(\mathbf{x},\mathbf{k}). \tag{3.4b}$$

Here $E(t,\mathbf{k})$ depends on $\mathbf{k}$ through (2.27) with $\omega(s)$ and $\kappa(s)$ being replaced with $\omega(s,\mathbf{k})$ and $\kappa(s,\mathbf{k})$, respectively.

Now, in order for ψ and $\bar{\psi}$ to be canonical, the wave functions u and $\bar{u}$ have to form a canonical complete set[6] that will be defined shortly. In the case of type 1 field, the simplest choice of U and $\overline{U}$,

$$U(\mathbf{x},\mathbf{k})^{\mu\nu} = [\delta^{\mu\nu}/(2\pi)^{3/2}] e^{i\mathbf{k}\cdot\mathbf{x}}, \tag{3.5a}$$

$$\overline{U}(\mathbf{x},\mathbf{k})^{\mu\nu} = [\delta^{\mu\nu}/(2\pi)^{3/2}] e^{-i\mathbf{k}\cdot\mathbf{x}}, \tag{3.5b}$$

turns out to give such a canonical set $\{u,\bar{u}\}$. We are going to show this below.

Since the thermal covariant derivatives $D^{+}(t)$ and $\overleftarrow{D}^{+}(t)$ in (2.31) depend on the momentum $\mathbf{k}$ we denote them by $D^{+}(t,\mathbf{k})$ and $\overleftarrow{D}^{+}(t,\mathbf{k})$. The field equations for ψ and $\bar{\psi}$ and those for u and $\bar{u}$ follow from (3.2)–(3.5) and (2.32),

$$iD^{+}(t,-i\nabla)^{\mu\nu}\psi(x)^{\nu} = 0, \tag{3.6a}$$

$$i\bar{\psi}(x)^{\nu}\overleftarrow{D}^{+}(t,i\overleftarrow{\nabla})^{\nu\mu} = 0, \tag{3.6b}$$

$$iD^{+}(t,\mathbf{k})^{\mu\lambda} u(x,\mathbf{k})^{\lambda\nu} = 0, \tag{3.6c}$$

$$i\bar{u}(x,\mathbf{k})^{\nu\lambda}\overleftarrow{D}^{+}(t,\mathbf{k})^{\lambda\mu} = 0. \tag{3.6d}$$

Using (3.4) and (3.5), we can prove that u and $\bar{u}$ satisfy the *orthonormalization relation*

$$\int d^3x\, \bar{u}(x,\mathbf{k}) u(x,l) = \delta(\mathbf{k}-l) \tag{3.7}$$

at any time t.

Furthermore, we can explicitly prove the sum rule

$$G^{+}(x,x')^{\mu\nu} = \int d^3k\, u(x,\mathbf{k})^{\mu\lambda} \bar{u}(x',\mathbf{k})^{\lambda\nu}, \tag{3.8}$$

where

$$G^{+}(x,x')^{\mu\nu} = \int \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \times [B^{-1}(t,\mathbf{k}) E(t,\mathbf{k}) E^{-1}(t',\mathbf{k}) B(t',\mathbf{k})]^{\mu\nu}. \tag{3.9}$$

The function $G^{+}(x,x')^{\mu\nu}$ has the following properties:

$$G^{+}(x,x')^{\mu\nu}\delta(t-t') = \delta^{\mu\nu}\delta^{(4)}(x-x'), \tag{3.10a}$$

$$iD^{+}(t,-i\nabla)^{\mu\lambda} G^{+}(x,x')^{\lambda\nu} = 0, \tag{3.10b}$$

$$iG^{+}(x,x')^{\nu\lambda}\overleftarrow{D}^{+}(t',i\overleftarrow{\nabla}')^{\lambda\mu} = 0. \tag{3.10c}$$

When u and $\bar{u}$ satisfy the orthonormalization conditions (3.7) and the sum rule (3.8) in which the function $G^{+}(x,x')$ has the properties in (3.10), the set $\{u,\bar{u}\}$ is called the *canonical complete set*. Using the properties of the canonical complete set, we obtain the equal-time canonical commutation relation

$$[\psi(t,\mathbf{x})^{\mu}, \bar{\pi}(t,\mathbf{x}')^{\nu}] = i\delta^{\mu\nu}\delta(\mathbf{x}-\mathbf{x}'), \tag{3.11}$$

where

$$\bar{\pi}(x) = i\bar{\psi}(x) \tag{3.12}$$

is the canonical conjugate of $\psi(x)$. This is the reason for the name "canonical complete set."

The semifree field equations in (3.6) can be derived from the following Lagrangian density:

$$\hat{\mathscr{L}}^{0}(x) = i\bar{\psi}(x)^{\mu} D^{+}(t,-i\nabla)^{\mu\nu}\psi(x)^{\nu}. \tag{3.13}$$

The momentum field $\bar{\pi}$ conjugate to ψ, already mentioned above, is indeed given by

$$\bar{\pi}(x)^{\mu} = \partial\hat{\mathscr{L}}^{0}(x)/\partial\dot{\psi}(x)^{\mu} = i\bar{\psi}(x)^{\mu}, \tag{3.14}$$

which is consistent with (3.12). The usual Legendre transformation gives us the semifree field Hamiltonian $\hat{H}_a^0$,

$$\hat{H}_a^0(t) = \int d^3x [\bar{\pi}\dot{\psi} - \hat{\mathscr{L}}^{0}] = \int d^3x\, \bar{\psi}(x)^{\mu} [\omega(t,-i\nabla) - iP(t,-i\nabla)]^{\mu\nu}\psi(x)^{\nu}, \tag{3.15}$$

where use was made of (2.33) in which $\omega(t)$ and $P(t)$ depend on $\mathbf{k}$ as $\omega(t,\mathbf{k})$ and $P(t,\mathbf{k})$, respectively. Needless to say, $\hat{H}_a^0$ is reduced to (2.42) when it is rewritten in terms of oscillator variables, $a(t,\mathbf{k})$ and $\bar{a}(t,\mathbf{k})$.

Here some comments on the semifree fields in the time-dependent case may be in order. As it was pointed out in Sec. II the generalized Bogoliubov transformation contains two arbitrary parameters, $b_L(t,\mathbf{k})$ and $b_R(t,\mathbf{k})$. Since the physical results are independent of these quantities we expect that these quantities do not cause any ambiguity in the choice of the Lagrangian. When we change these quantities ψ changes into ψ' and, at the same time, the expression for the Lagrangian density changes from $\mathscr{L}$ to $\mathscr{L}'$. However, the Lagrangian density is really unique in the sense that

$$\mathscr{L}'(\psi') = \mathscr{L}(\psi). \tag{3.16}$$

Then the canonical momenta of ψ and ψ' are given by $\bar{\pi} = \partial\mathscr{L}/\partial\dot{\psi}$ and $\bar{\pi}' = \partial\mathscr{L}'/\partial\dot{\psi}'$, respectively. Thus the Hamiltonian densities for ψ and ψ' are $[\bar{\pi}\dot{\psi} - \mathscr{L}]$ and $[\bar{\pi}'\dot{\psi}' - \mathscr{L}']$. The transformation $(\psi,\bar{\pi}) \to (\psi',\bar{\pi}')$ is a canonical transformation. For example, when $b_R(t)$ is changed to $b'_R(t)$, we have

$$\hat{H}_a^{0\prime}(t) - \hat{H}_a^0(t) = -i\int d^3k\, \bar{a}(t,\mathbf{k})^{\mu}\left[\partial_t\left\{\ln\frac{b'_R(t,\mathbf{k})}{b_R(t,\mathbf{k})}\right\}\tau_3\right]^{\mu\nu} a(t,\mathbf{k})^{\nu}. \tag{3.17}$$

The causal two-point function has the form

$$\Delta_c(x,x')^{\mu\nu} = -i\langle 0|T[\psi(x)^\mu\bar{\psi}(x')^\nu]|0\rangle \tag{3.18}$$

$$= [B^{-1}(t,-i\nabla)\mathcal{G}_c(x,x')B(t',\overleftarrow{i\nabla'})]^{\mu\nu}, \tag{3.19}$$

with

$$\mathcal{G}_c(x,x')^{11} = -i\theta(t-t')\int\frac{d^3k}{(2\pi)^3}e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \times\exp\left[-i\int_{t'}^{t}ds\{\omega(s,\mathbf{k})-i\kappa(s,\mathbf{k})\}\right], \tag{3.20a}$$

$$\mathcal{G}_c(x,x')^{22} = i\theta(t'-t)\int\frac{d^3k}{(2\pi)^3}e^{i\mathbf{k}\cdot(\mathbf{x}-\mathbf{x}')} \times\exp\left[-i\int_{t'}^{t}ds\{\omega(s,\mathbf{k})+i\kappa(s,\mathbf{k})\}\right], \tag{3.20b}$$

$$\mathcal{G}_c(x,x')^{12} = \mathcal{G}_c(x',x)^{21} = 0. \tag{3.20c}$$

In practical computations using the Feynman-diagram method we need the knowledge of the Feynman function and the interaction Hamiltonian in the interaction representation. The Feynman function is given by $\Delta_c(x,x')$ in (3.19). The interaction Hamiltonian will be studied in the next section.

IV. THE INTERACTION HAMILTONIAN

Assuming a given system, we denote its Lagrangian density by $\mathcal{L}$. Then we can construct $\tilde{\mathcal{L}}$ by means of the tilde conjugation rules. It has been shown that the total Lagrangian density in TFD is

$$\hat{\mathcal{L}} = \mathcal{L} - \tilde{\mathcal{L}}. \tag{4.1}$$

Different thermal situations are covered by the different realizations of operators satisfying the field equation which follows from $\hat{\mathcal{L}}$. As it was pointed out above, when we deal with time-dependent thermal situations the Hamiltonian depends on the choice of field variables, while the Lagrangian does not. In other words $\hat{\mathcal{L}}$ is independent of the thermal situation. Therefore use of the Lagrangian is more suitable for the unambiguous definition of the interaction than use of the Hamiltonian.

Let us consider the following Lagrangian density for an unrenormalized bosonic complex field ψ_0:

$$\mathcal{L}(\psi_0) = \psi_0^*[i\partial_t - \omega_0]\psi_0 - g_0 W(\psi_0^*\psi_0). \tag{4.2}$$

Here $W(x)$ is a polynomial function of x and the subscript 0 means unrenormalized quantities. According to the tilde conjugation rules we have the total Lagrangian density $\hat{\mathcal{L}}$ in TFD as follows:

$$\hat{\mathcal{L}} = \mathcal{L} - \tilde{\mathcal{L}} = \bar{\psi}_0(x)^\mu[i\partial_t - \omega_0(i\nabla)]\psi_0(x)^\mu - g_0\{W(\bar{\psi}_0(x)^1\psi_0(x)^1) - W(-\bar{\psi}_0(x)^2\psi_0(x)^2)\}, \tag{4.3}$$

where the thermal doublet notation is made use of. The bare quantities should be related to renormalized ones through the renormalization transformations. In addition to the energy renormalization

$$\omega_0 = \omega - \delta\omega, \tag{4.4}$$

where ω is the renormalized energy and $\delta\omega$ is the self-energy, we consider also the wave function renormalization. In TFD the wave function renormalization factor can be a 2×2 matrix that will be denoted by V, with V being a 2×2 matrix. Thus the wave function renormalization reads as

$$\psi_0(x)^\mu = V(t)^{\mu\nu}\psi(x)^\nu, \tag{4.5a}$$

$$\bar{\psi}_0(x)^\mu = \bar{\psi}(x)^\nu V^{-1}(t)^{\nu\mu}. \tag{4.5b}$$

We consider this wave function renormalization by requiring that V is diagonal, i.e.,

$$V(t)^{\mu\nu} = V(t;\tau_3)^{\mu\nu}. \tag{4.6}$$

The reason for this will become clear shortly. In this paper we do not discuss the coupling constant renormalization and the overall wave function renormalization other than V.

Substituting (4.4) and (4.5) into (4.3) we have $\hat{\mathcal{L}}$ expressed in terms of the renormalized quantities

$$\hat{\mathcal{L}} = \hat{\mathcal{L}}^0 + \hat{\mathcal{L}}_{\text{int}}, \tag{4.7}$$

$$\hat{\mathcal{L}}^0 = \bar{\psi}^\mu[i\partial_t - \omega + iP]^{\mu\nu}\psi^\nu, \tag{4.8}$$

$$\hat{\mathcal{L}}_{\text{int}} = -g_0\{W(Z_3\bar{\psi}^1\psi^1) - W(-Z_3\bar{\psi}^2\psi^2)\} + \bar{\psi}^\mu[iV^{-1}\dot{V} + \delta\omega - iP]^{\mu\nu}\psi^\nu, \tag{4.9}$$

where $P(t)$ was given in (2.34). Comparing (4.8) with (3.13) and (2.33a) we see that the unperturbed Lagrangian density $\hat{\mathcal{L}}^0$ in (4.7) is the semifree field Lagrangian density in (3.13). Note that iP in $\hat{\mathcal{L}}^0$ and iP in $\hat{\mathcal{L}}_{\text{int}}$ cancel one another. The total Hamiltonian follows from (4.7) as

$$\hat{H} = \hat{H}_a^0 + \hat{H}_{\text{int}}, \tag{4.10}$$

where $\hat{H}_a^0$ was given in (3.15) and

$$\hat{H}_{\text{int}} = \int d^3x[g_0\{W(\bar{\psi}^1\psi^1) - W(-\bar{\psi}^2\psi^\nu)\} - \bar{\psi}^\mu[iV^{-1}\dot{V} + \delta\omega - iP]^{\mu\nu}\psi^\nu] \tag{4.11}$$

$$= \int d^3x[g_0\{W(\bar{\psi}^1\psi^1) - W(-\bar{\psi}^2\psi^2)\} - \bar{\psi}^\mu[iV^{-1}\dot{V} + \delta\omega - i(\kappa A + \dot{n}\tau) - iW_R^{-1}\dot{W}_R]^{\mu\nu}\psi^\nu], \tag{4.12}$$

where (2.34)–(2.36) are considered. Without loss of generality we can choose

$$V = W_R. \tag{4.13}$$

This gives

$$V^{-1}\dot{V} - W_R^{-1}\dot{W}_R = 0. \tag{4.14}$$

According to (2.20c), this makes V diagonal. Now the inter-

action Hamiltonian is

$$\hat{H}_{\text{int}} = \int d^3x[\, g_0\{W(\bar{\psi}^1\psi^1) - W(-\bar{\psi}^2\psi^2)\} - \bar{\psi}^\mu[\delta\omega(t) - i\{\kappa(t)A(t) + \dot{n}(t)\tau(t)\}]^{\mu\nu}\psi^\nu], \tag{4.15}$$

$$= \int d^3x[\, g_0\{W(\bar{\psi}^1\psi^1) - W(-\bar{\psi}^2\psi^2)\} - [\bar{\psi}W_R^{-1}(t)]^\mu[\delta\omega(t) - i\{\kappa(t)A_0(t) + \dot{n}(t)\tau_0\}]^{\mu\nu}[W_R(t)\psi]^\nu], \tag{4.16}$$

where (2.38) and (2.40) were used. Note that A_0 and τ_0 were given in (2.39) and (2.41), respectively.

With the knowledge of this interaction Hamiltonian and the casual two-point function of the semifree field in (3.19), we can formulate the perturbative computation in terms of the Feynman diagrams. A vital step in this formulation is the renormalization procedure which leads to the self-consistent equations for ω, κ, and n. This will be illustrated in the next section by means of a simple model. There, an explicit form of the on-shell renormalization condition is presented. We will see also how the self-consistent equation determines the time dependence of $n(t)$ when the initial value n $(t=0)$ is given.

V. EXAMPLE OF TIME-DEPENDENT RENORMALIZATION—THE THERMAL RESERVOIR MODEL

In this section we illustrate the self-consistent renormalization method by taking as an example the well-known thermal reservoir model, which is a system with a thermal reservoir. We treat the entire system including the reservoir as one system. Therefore this example shows explicitly how dissipation is created spontaneously. The explicit calculation below will also indicate how the self-consistent renormalization method should be formulated in time-dependent situations.

The model consists of a simple harmonic oscillator $(a,a^\dagger)$ and a reservoir $(R_k,R_k^\dagger;\ k=1,2,...,N)$ interacting with each other. These operators satisfy

$$[a,a^\dagger]_\sigma = 1, \tag{5.1a}$$

$$[R_k,R_l^\dagger]_\sigma = \delta_{kl}. \tag{5.1b}$$

The total Hamiltonian H is assumed to take the simple bilinear form

$$H = \omega_0 a^\dagger a + \sum_{k=1}^{N} \Omega_{0k} R_k^\dagger R_k + g\sum_{k=1}^{N}(R_k^\dagger a + a^\dagger R_k), \quad \text{with } N\to\infty. \tag{5.2}$$

According to the usual notion of a reservoir, g^2 is of order $1/N$,

$$\bar{g}^2 = Ng^2. \tag{5.3}$$

The spacing of reservoir energy levels is of order $1/N$,

$$\Omega_{0k} = \bar{\Omega}_0 + k\delta; \quad \delta = O(1/N), \tag{5.4}$$

and the bandwidth Δ of the reservoir energy spectrum is given by

$$\Delta = N\delta. \tag{5.5}$$

Note that the limit $N\to\infty$ should be performed at the end of computation, because otherwise the $(R_k,R_k^\dagger)$ system cannot act as a thermal reservoir. At this limit the energy spectrum Ω_{0k} becomes a continuum. We have previously treated this model in the stationary case.[5] There the $(1/N)$-power expansion was made. With each finite order in this expansion a dissipation does appear. When N is finite we should sum up all of the $(1/N)$-power expansion terms and then the dissipation simply disappears (i.e., $\kappa=0$). However, since N is infinite only the leading term in the $(1/N)$-power expansion should be picked up. Then a dissipative effect remained (i.e., $\kappa\neq 0$).

Physically, the spontaneously created dissipation is a result of decay processes of the oscillator into the reservoir quanta through infinite channels, the decay probability for each channel being infinitesimal. This decay is the thermal instability that is encouraged by the negative energy of the tilde quanta. Thus the infinite degrees of freedom together with the negative energy of the tilde quanta is the origin of the spontaneous creation of dissipation. The role played by the infinite degrees of freedom is the same as the one in the phenomena of spontaneous breakdown of symmetries which require the infinite degrees of freedom.[8] We might say that the system behaves like an "open" system, not because of the elimination of reservoir variables (which we do not do), but because each decay product appearing with infinitesimal probability is not observable. The situation is very similar to the case of impurity scattering because the unobservable tilde quanta act like the impurities. In other words, the dissipation is caused by the communication of nontilde quanta with the unobservable background field which is the tilde field. Intuitively this tilde field effect represents the effect of thermally excited particles. It could be that this process may act as the coarse graining.

In previous papers[5] we studied only the time-independent situation. The result agreed fully with the well-known result of the projection operator method applied to the Liouville equation for the density matrix. Although the thermal averages are time independent, any two-point function or correlation function has a dissipative effect, which is a manifestation of the contributions from the excited states dissipatively approaching the equilibrium state. The number distribution of the oscillator was found to be $n = 1/[e^{\beta\omega} - \sigma]$ with $\beta = 1/k_B T$, with T being the temperature of the reservoir. This was a result of the self-consistent equations obtained by the renormalization method. Therefore we may expect that when we prepare the initial value of $n(t)$ different from $1/[e^{\beta\omega} - \sigma]$, n should become dependent on time. The temporal behavior of $n(t)$ should also be determined by the self-consistent renormalization method. Thus our consideration in this section presents the *renormalization condition for time-dependent thermal phenomena* which has never previously been presented. With the help of the considerations in the previous sections we are now ready to treat the model (5.2) in a time-dependent situation.

Since the $(R_k,R_k^\dagger)$ system is a reservoir it should be in

an equilibrium state and have the number distribution

$$n_k = [e^{\beta\Omega_k} - \sigma]^{-1}, \tag{5.6}$$

with Ω_k being the renormalized energy. On the other hand, the initial value (i.e., the value of $t = 0$) of the number distribution $n(t)$ of the $(a,a^\dagger)$ oscillator is not specified.

According to (2.42) the unperturbed semifree Hamiltonian is

$$\hat{H}^0(t) = \bar{a}(t)^\mu[\omega - iP(t)]^{\mu\nu}a(t)^\nu + \sum_{k=1}^{N} \bar{R}_k(t)^\mu[\Omega_k - iP_k]^{\mu\nu}R_k(t)^\nu. \tag{5.7}$$

Since Ω_k and P_k are time independent (2.34) together with (2.20), (2.38), and (2.39) gives

$$P_k = \kappa_k A_k \tag{5.8}$$

with

$$A_k = W_{Rk}^{-1}A_{0k}W_{Rk}, \tag{5.9}$$

$$A_{0k} = \begin{bmatrix} 1+2\sigma n_k & -2\sigma n_k \\ 2(1+\sigma n_k) & -(1+2\sigma n_k) \end{bmatrix}, \tag{5.10}$$

$$W_{Rk} = e^{\tau_3 \ln b_{Rk}}. \tag{5.11}$$

The $P(t)$ was given in (2.34).

We assume that the wave function renormalization (4.5) with $V = W_R$ [cf. (4.13)] has already been performed. Then the interaction Hamiltonian is given by (4.16),

$$\begin{aligned}\hat{H}_{\text{int}} = g\sum_{k=1}^{N} &\{\bar{R}_k(t)^\mu[W_{Rk}^{-1}W_R(t)]^{\mu\nu}a(t)^\nu \\ &+ \bar{a}(t)^\mu[W_R^{-1}(t)W_{Rk}]^{\mu\nu}R_k(t)^\nu\} \\ &- [\bar{a}(t)W_R^{-1}(t)]^\mu[\delta\omega - i\{\kappa A_0(t) + \sigma\dot{n}(t)\tau_0\}]^{\mu\nu} \\ &\times[W_R(t)a(t)]^\nu \\ &- \sum_{k=1}^{N}[\bar{R}_k(t)W_{Rk}^{-1}]^\mu[\delta\Omega_k - i\kappa_k A_{0k}]^{\mu\nu} \\ &\times[W_{Rk}R_k(t)]^\nu.\end{aligned} \tag{5.12}$$

Note that according to (2.35) $\dot{n}(t)$ should carry the factor σ.

We first assume that ω and κ are independent of time. We are going to justify this assumption by showing that it is consistent with the self-consistent equation which will be derived shortly.

The casual two-point functions are

$$\Delta_c(t_1,t_2)^{\mu\nu} = -i\langle 0|T[a(t_1)^\mu\bar{a}(t_2)^\nu]|0\rangle, \tag{5.13}$$

$$= [B^{-1}(t_1)\varphi(t_1-t_2)B(t_2)]^{\mu\nu}, \tag{5.14}$$

$$\Delta_{ck}(t_1,t_2)^{\mu\nu}\delta_{kl} = -i\langle 0|T[R_k(t_1)^\mu\bar{R}_l(t_2)^\nu]|0\rangle, \tag{5.13'}$$

$$= [B_k^{-1}\varphi_k(t_1-t_2)B_k]^{\mu\nu}\delta_{kl}, \tag{5.14'}$$

where

$$\varphi(t_1-t_2)^{11} = -i\theta(t_1-t_2)\exp[-i(\omega - i\kappa)(t_1-t_2)], \tag{5.15a}$$

$$\varphi(t_1-t_2)^{22} = i\theta(t_2-t_1)\exp[-i(\omega + i\kappa)(t_1-t_2)], \tag{5.15b}$$

$$\varphi_k(t_1-t_2)^{11} = -i\theta(t_1-t_2)\exp[-i(\Omega_k - i\kappa_k)(t_1-t_2)], \tag{5.15c}$$

$$\varphi_k(t_1-t_2)^{22} = i\theta(t_2-t_1)\exp[-i(\Omega_k + i\kappa_k)(t_1-t_2)], \tag{5.15d}$$

$$\varphi(t_1-t_2)^{\mu\nu} = \varphi_k(t_1-t_2)^{\mu\nu} = 0, \quad \text{for } \mu \neq \nu. \tag{5.15e}$$

It can be seen from (5.12) that the computation is very much simplified when we choose the arbitrary matrix W_R to be independent of time. This choice corresponds to taking a time-dependent α because $n(t)$ or $f(t)$ change with time [see (2.20c), (2.23)–(2.25)]. Then the proper self-energy diagram for $(a,\bar{a})$ gives

$$\begin{aligned}\Sigma(t_1,t_2)^{\mu\nu} = W_R^{-1\mu\lambda}&\left[g^2\left\{\sum_{k=1}^{N} W_{Rk}\Delta_{ck}(t_1-t_2)W_{Rk}^{-1}\right\}\right. \\ &\left. - \{\delta\omega - i(\kappa A_0(t_1) + \sigma\dot{n}(t_1)\tau_0)\}\delta(t_1-t_2)\right]^{\lambda\rho}W_R^{\rho\nu},\end{aligned} \tag{5.16}$$

while the one for $(R_k,\bar{R}_k)$ is

$$\begin{aligned}\Sigma_k(t_1,t_2)^{\mu\nu} = W_{Rk}^{-1\mu\lambda}&[g^2\{W_R\Delta_c(t_1,t_2)W_R^{-1}\} \\ &- \{\delta\Omega_k - i\kappa_k A_{0k}\}\delta(t_1-t_2)]^{\lambda\rho}W_{Rk}^{\rho\nu}.\end{aligned} \tag{5.17}$$

The connected full propagators of a and R_k (i.e., G and G_k) satisfy the following Dyson equations:

$$G(t_1,t_2) = \Delta_c(t_1,t_2) + \int ds_1\,ds_2\,\Delta_c(t_1,s_1)\Sigma(s_1,s_2)G(s_2,t_2), \tag{5.18a}$$

$$G_k(t_1,t_2) = \Delta_{ck}(t_1,t_2) + \int ds_1\,ds_2\,\Delta_{ck}(t_1-s_1)\Sigma_k(s_1,s_2)G_k(s_2,t_2). \tag{5.18b}$$

The self-energies above are functions of two times, t_1 and t_2. As a result of this we cannot directly follow the same procedure for the on-shell renormalization as in the stationary case or in the usual quantum field theory.

In the present model, the *on-shell renormalization conditions* of Σ and Σ_k are stated as follows:

$$\Sigma(\omega,k_0) = 0, \tag{5.19a}$$

$$\Sigma(k_0,\omega) = 0, \tag{5.19b}$$

$$\Sigma_k(\Omega_k,k_0) = 0, \tag{5.19c}$$

$$\Sigma_k(k_0,\Omega_k) = 0, \tag{5.19d}$$

for arbitrary real k_0. Here the Fourier transform of any two-time function [say $f(t_1,t_2)$] is defined by

$$f(k_0^1,k_0^2) = \int\int dt_1\,dt_2\,e^{ik_0^1t_1}f(t_1,t_2)e^{-ik_0^2t_2}. \tag{5.20}$$

These on-shell renormalization conditions are equivalent to

$$\Sigma(\omega,t) = 0, \tag{5.21a}$$

$$\Sigma(t,\omega) = 0, \tag{5.21b}$$

$$\Sigma_k(\Omega_k,t) = 0, \tag{5.21c}$$

$$\Sigma_k(t,\Omega_k) = 0, \tag{5.21d}$$

at any time t.

When (5.16) and (5.17) are considered, (5.21a) and (5.21c) read as

$$W_R\Sigma(\omega,t)W_R^{-1} = e^{i\omega t}\left[\frac{\bar{g}^2}{N}\sum_{k=1}^{N}\frac{1}{(\omega-\Omega_k)+i\kappa_k A_{0k}} - \delta\omega + i(\kappa A_0(t)+\sigma\dot{n}(t)\tau_0)\right]=0, \tag{5.22a}$$

$$W_{Rk}\Sigma_k(\Omega_k,t)W_{Rk}^{-1} = \frac{\bar{g}^2}{N}W_R\left[\int ds\, e^{i\Omega_k s}B^{-1}(s)g(s-t)B(t)\right]W_R^{-1} - e^{i\Omega_k t}[\delta\Omega_k - i\kappa_k A_{0k}]=0, \tag{5.22b}$$

with (5.3) and (5.14).

Equation (5.22b) is the self-consistent equation for $\delta\Omega_k$ and κ_k. This leads to the vanishing of $\delta\Omega_k$ and κ_k when N is taken to infinite with fixed $\bar{g}^2$,

$$\delta\Omega_k = O(1/N), \tag{5.23a}$$

$$\kappa_k = O(1/N). \tag{5.23b}$$

This situation is the same as the one in the stationary case studied previously. On the other hand, dividing another self-consistent equation (5.22a) into real and imaginary parts, we have the matrix equations,

$$\kappa A_0(t)+\sigma\dot{n}(t)\tau_0 = \frac{\bar{g}^2}{N}\sum_{k=1}^{N}\frac{\kappa_k}{(\omega-\Omega_k)^2+\kappa_k^2}A_{0k}, \tag{5.24a}$$

$$\delta\omega = \frac{\bar{g}^2}{N}\sum_{k=1}^{N}\frac{(\omega-\Omega_k)}{(\omega-\Omega_k)^2+\kappa_k^2}, \tag{5.24b}$$

using the property $A_{0k}^2=1$. Equation (5.24b) again has the same expression as the one in the stationary case studied in Ref. 5.

Let us now solve (5.24a) at the limit $N\to\infty$. Then Ω_k becomes a continuous parameter denoted by Ω and summation becomes integration,

$$\kappa A_0(t)+\sigma\dot{n}(t)\tau_0 = \frac{\bar{g}^2}{\Delta}\int_\Delta d\Omega\,\pi\delta(\omega-\Omega)A_{0R}(\Omega) = \frac{\pi\bar{g}^2}{\Delta}A_{0R}(\omega), \tag{5.25}$$

where $A_{0R}(\Omega)$ is A_{0k} in (5.10) with n_k being replaced with [cf. (5.6)],

$$n_R(\Omega) = [e^{\beta\Omega}-\sigma]^{-1}. \tag{5.26}$$

Let us introduce $\bar{n}$ by

$$\bar{n} = n_R(\omega) = [e^{\beta\omega}-\sigma]^{-1}. \tag{5.27}$$

Then

$$A_{0R}(\omega) = \begin{bmatrix} 1+2\sigma\bar{n} & -2\sigma\bar{n} \\ 2(1+\sigma\bar{n}) & -(1+2\sigma\bar{n})\end{bmatrix}. \tag{5.28}$$

Now recall (2.39) and (2.41), i.e.,

$$A_0(t) = \begin{bmatrix} 1+2\sigma n(t) & -2\sigma n(t) \\ 2(1+\sigma n(t)) & -(1+2\sigma n(t))\end{bmatrix}, \tag{5.29}$$

$$\tau_0 = \begin{bmatrix} 1 & -1 \\ 1 & -1\end{bmatrix}. \tag{5.30}$$

The four matrix elements of the self-consistent equation (5.25) give the following three equations:

$$\kappa\{1+2\sigma n(t)\}+\sigma\dot{n}(t) = (\pi\bar{g}^2/\Delta)\{1+2\sigma\bar{n}\}, \tag{5.31a}$$

$$2\sigma\kappa n(t)+\sigma\dot{n}(t) = (\pi\bar{g}^2/\Delta)2\sigma\bar{n}, \tag{5.31b}$$

$$2\kappa\{1+\sigma n(t)\}+\sigma\dot{n}(t) = (\pi\bar{g}^2/\Delta)2\{1+\sigma\bar{n}\}. \tag{5.31c}$$

However the addition of (5.31b) and (5.31c) leads to (5.31a), which implies that the independent equations are any two of (5.31a)–(5.31c). They give

$$\kappa = \pi\bar{g}^2/\Delta, \tag{5.32a}$$

$$\dot{n}(t) = -2\kappa[n(t)-\bar{n}]. \tag{5.32b}$$

The dissipative factor κ is found to be the same as in the stationary case.[5] When the initial value of $n(t)$ is given by $n(0)$, (5.32b) determines the temporal behavior of $n(t)$,

$$n(t) = [n(0)-\bar{n}]e^{-2\kappa t}+\bar{n}. \tag{5.33}$$

This leads to

$$n(\infty) = \bar{n}. \tag{5.34}$$

Then (5.27) indicates that $n(t)$ in (5.33) starts with the initial value $n(0)$ and approaches the equilibrium value $n_R(\omega)$ at $t\to\infty$.

The fact that $\kappa\neq 0$ indicates the spontaneous creation of dissipation.

Note that the substitution of the solutions of the self-consistent equation rewrite $\hat{H}^0(t)$ in (5.7) as the following form for the final equilibrium situation:

$$\hat{H}^0(t) = \bar{a}(t)^\mu[\omega-i\bar{P}]^{\mu\nu}a(t)^\nu + \sum_{k=1}^{N}\bar{R}_k(t)^\mu\Omega_k R_k(t)^\mu, \tag{5.35}$$

where

$$\bar{P} = \kappa A_{0R}(\omega). \tag{5.36}$$

Thus the reservoir model is described by the time-independent Hamiltonian for equilibrium. But this may not be true when the higher-order corrections are taken account of in general nonlinearly interacting systems.

When we happen to choose $n(0)=\bar{n}$ then $n(t)$ becomes independent of time and we have the equilibrium situation. This is the case studied in Ref. 5.

We now comment on the Heisenberg operators. When we express the Heisenberg operators a_H^μ in terms of the interaction representation operator a^μ and R_k^μ, we find that

$$a_H(t)^\mu = e(t,0)a(t=0)^\mu - ig\sum_{k=1}^{N}\int_0^t dt_1\,\theta(t-t_1)e(t,t_1)R_k(t_1)^\mu, \tag{5.37a}$$

$$\bar{a}_H(t)^\mu = \bar{a}(t=0)^\mu e^*(0,t) + ig\sum_{k=1}^{N}\int_0^t dt_1\,\bar{R}_k(t_1)^\mu e^*(t_1,t)\theta(t-t_1), \tag{5.37b}$$

where $e(t,t_1)$ is a certain c-number function.[15] When $|a\rangle$ and $|b\rangle$ denote any two vectors in our Fock space and $g^2=\bar{g}^2/N$

is considered,

$$\lim_{N\to\infty}\langle a|a_H(t)^\mu|b\rangle=\langle a|e(t,0)a(t=0)^\mu|b\rangle, \tag{5.38a}$$

$$\lim_{N\to\infty}\langle a|\bar{a}_H(t)^\mu|b\rangle=\langle a|\bar{a}(t=0)^\mu e^*(0,t)|b\rangle, \tag{5.38b}$$

which means that $a_H^\mu(t)$ is weakly equal to $e(t,0)a^\mu(t=0)$,

$$a_H^\mu(t)\overset{W}{=}e(t,0)a^\mu(t=0),\quad \text{etc.} \tag{5.39}$$

However, this does not mean that $\bar{a}_H^\mu(t)a_H^\nu(t)$ is weakly equal to $|e(t,0)|^2\bar{a}^\mu(0)a^\nu(0)$ because the R_k^μ terms in (5.37) contribute to $\bar{a}_H^\mu(t)a_H^\nu(t)$ even at the limit $N\to\infty$.[16] It can be shown that $e(t,t_1)$ satisfies

$$[i\partial_t-\omega_0]e(t,t_1)+i\frac{\kappa}{\pi}\int_0^t dt_2\int_\Delta d\Omega\, e^{-i\Omega(t-t_2)}\theta(t_2-t_1)e(t_2,t_1)=0, \tag{5.40a}$$

with

$$e(t,t)=1. \tag{5.40b}$$

Since

$$F(t-t_1)=\int_\Delta d\Omega\, e^{-i\Omega(t-t_1)} \tag{5.41}$$

is a function that has a peak at $t=t_1$ and becomes very small for $|t-t_1|\gg 1/\Delta$, $e(t,t^1)$ can be approximately written as

$$e(t,t^1)\simeq e(t)e^{-1}(t_0), \tag{5.42}$$

when κ is small (i.e., Δ is large). Here $e(t)$ is a solution of the equation

$$(i\partial_t-\omega+i\kappa)e(t)=0 \tag{5.43a}$$

with

$$e(0)=1. \tag{5.43b}$$

Note that ω_0 is equal to ω in this approximation. Thus

$$e(t)=e^{-i\omega t-\kappa t}. \tag{5.44}$$

A calculation shows that

$$n_H(t)\simeq\langle 0|\bar{a}_H(t)^1a_H(t)^1|0\rangle=|e(t)|^2\left[n(0)+\frac{\kappa}{\pi}\int_0^t d\Omega\, n_R(\Omega)\left|\int_0^t dt_1\, e^{-i\Omega t_1}e^{-1}(t_1)\right|^2\right]. \tag{5.45}$$

Use of (5.45) gives

$$n_H(t)\simeq e^{-2\kappa t}\left[n(0)+\int d\Omega\,\rho(\Omega)n_R(\Omega)|e^{\kappa t-i(\omega-\Omega)t}-1|^2\right], \tag{5.46}$$

where

$$\rho(\Omega)=\frac{1}{\pi}\frac{\kappa}{(\omega-\Omega)^2+\kappa^2}. \tag{5.47}$$

We can rewrite (5.46) as

$$n_H(t)\simeq\bar{n}_R+e^{-2\kappa t}[n(0)-\bar{n}_R]+2e^{-\kappa t}\left[\bar{n}_R e^{-\kappa t}-\int_\Delta d\Omega\,\rho(\Omega)n_R(\Omega)\cos(\omega-\Omega)t\right], \tag{5.48}$$

where

$$\bar{n}_R=\int d\Omega\,\rho(\Omega)n_R(\Omega). \tag{5.49}$$

Since $\rho(\Omega)$ is a function whose peak is at $\Omega=\omega$ and whose width is κ, $\bar{n}_R$ is very close to $\bar{n}$ when κ is small. Equation (5.48) indicates that $n_H(t=\infty)=\bar{n}_R$ and $n_H(t=0)=n(0)$, behaving like $n(t)$ at $t=\infty$ and $t=0$. The last bracket term in (5.48) gives the difference between $n_H(t)$ and $n(t)$ when t is finite and nonvanishing. Since $\Delta\gg\kappa$, the presence of $\rho(\Omega)$ makes the last integral term vanish quickly at $t\gg 1/\kappa$. When Δ is large and κ is small, $n_H(t)$ and $n(t)$ behave similarly. At present, we are not sure which one should correspond to the observable value. We might consider also the quantity

$$N_H(t)={}_H\langle 0|\bar{a}_H(t)^1a_H(t)^1|0\rangle_H$$

with

$$|0\rangle_H=u(0,-\infty)|0\rangle/[\langle 0|u(\infty,-\infty)|0\rangle]^{1/2}$$

and

$${}_H\langle 0|=\langle 0|u(\infty,0)/[\langle 0|u(\infty,-\infty)|0\rangle]^{1/2}.$$

We then find

$$N_H(t)=\langle 0|u(\infty,t)\bar{a}(t)^1a(t)^1u(t,-\infty)|0\rangle\times\langle 0|u(\infty,-\infty)|0\rangle^{-1}. \tag{5.50}$$

Since $u(0,-\infty)|0\rangle$ may make $|0\rangle_H$ equilibrium, $N_H(t)$ is the average number in the equilibrium state. This can be confirmed by means of an explicit computation. It is still an important open question as to what really corresponds to each observable quantity. We are planning to continue our study by assuming that $n(t)$ describes the behavior of number in a reasonable approximation.

We discussed the Heisenberg operators in the reservoir model, but we should be careful not to extend the arguments to general nonlinearly interacting systems in which the dynamical maps may be very complicated. The problem of the Heisenberg operator in general models of time-dependent TFD is still unsolved.

VI. SUMMARY

We have presented a general formalism for semifree field theory which includes the time-dependent thermal situation. The formalism expressed in terms of oscillator operators was given in Sec. II. The formalism expressed in terms of field operators was presented in Sec. III. It is due to a complication caused by the time-dependent nature of the thermal behavior that the consideration in Sec. III was limited to the semifree field of type 1. In the Appendix we discuss the semifree field of type 2 in a stationary situation. Using the knowledge of the total Lagrangian in TFD and choosing the semifree field Lagrangian for the unperturbed Lagrangian, we

determined the general form of the interaction Hamiltonian, in the interaction representation, for any time-dependent situation in Sec. IV. This is the basis for the Feynman-type perturbative calculation in TFD in time-dependent situations. A set of self-consistent equations determine ω_k, κ_k, and the temporal behavior of the average number density $n_k(t)$. An example of the derivation of the self-consistent equations in a time-dependent situation was studied in Sec. V. A remarkable point in this consideration is the explicit expression of the *on-shell renormalization condition* in the time-dependent situation which leads to the self-consistent equations. The latter equations were explicitly solved, and κ and $n(t)$ were determined.

Since $n(t) = \langle 0|\bar{a}(t)^1 a(t)^1|0\rangle$, the explicit t dependence of n indicates that the time-translational symmetry (based on $\hat{H}|0\rangle = 0$) is spontaneously broken. This is a result of the communication between the nontilde quanta with the background tilde field which is a manifestation of the effects of the thermally excited quanta which have infinite degrees of freedom. This communication seems to be playing a role similar to the coarse graining. The negative sign of the energy of the tilde quanta encourage the thermal instability, leading to the dissipation. Since there are an infinite number of dissipative channels, each of which participates with infinitesimal probability, the instability takes the form of dissipation. This becomes clear through the example in Sec. V when the $(1/N)$-power expansion method (N: number of degrees of freedom) with the limit $N \to \infty$.

The spontaneous breakdown of the time-translation symmetry suggests that, at any finite time, there are no eigenvectors of the basic total Hamiltonian $\hat{H} = H - \tilde{H}$ in our representation space, which is the Fock space of $\xi(0)^\mu$ and $\bar{\xi}(0)^\mu$. The diagonal property of the time-translation matrix $E_0(t)$ in (2.10) implies that the realization space remains unchanged during the time evolution. However, the dynamical map of $\hat{H}$ expressed in terms of quasiparticle operators depends on time explicitly. In this sense, the realization of $\hat{H}$ depends on time. As a matter of fact, when a system reaches an equilibrium state, the thermal vacuum may become an eigenvector of $\hat{H}$ at $t = \infty$. Then the time-translation symmetry may be recovered at $t \to \infty$, although κ does not vanish at $t = \infty$. (Remember that κ is independent of time in Sec. V.)

Here a comment about the quasiparticle number may be in order. Although $n(t) = \langle 0|\bar{a}(t)^1 a(t)^1|0\rangle$ is the number of the unperturbed particles, *this includes all of the loop corrections*, because the unperturbed particle is the quasiparticle that is *fully normalized*. Each loop correction in the self-energy diagram modifies the parameters such as ω, κ, and $n(t)$ in the unperturbed Hamiltonian through the self-consistent renormalization condition.

Although the consideration in Sec. V is the first explicit treatment of the on-shell time-dependent renormalization condition, this consideration is still simple in the sense that ω and κ are independent of time. When we study a transition from temperature T to T', and when the quantum energy depends on temperature, it is obvious that the energy ω changes in time. A study of such a case requires the most complete form of the on-shell time-dependent renormalization condition. We are planning an application of the formalism in this paper to a case in which ω and κ depend on time. A strong merit of TFD presented in this paper is that it can be applied to any thermal situation including an isolated dynamical system. Thus TFD is suitable for treating the thermal behavior of the Universe.

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APPENDIX: THE SEMIFREE FIELDS OF TYPE 2 IN THE TIME-INDEPENDENT SITUATION

In Sec. II we considered the wave functions $u(x,\mathbf{k})$ with the positive frequency. The equation for $u(x,\mathbf{k})$ was summarized in (3.6),

$$iD^+(t,\mathbf{k})^{\mu\nu}u(x,\mathbf{k})^\nu = 0, \tag{A1a}$$

$$i\bar{u}(x,\mathbf{k})^\nu \overleftarrow{D}^+(t,\mathbf{k})^{\nu\mu} = 0. \tag{A1b}$$

The thermal covariant derivatives were defined in (2.31),

$$D^+(t,\mathbf{k}) = B^{-1}(t,\mathbf{k})E(t,\mathbf{k})\partial_t E^{-1}(t,\mathbf{k})B(t,\mathbf{k}), \tag{A2a}$$

$$\overleftarrow{D}^+(t,\mathbf{k}) = B^{-1}(t,\mathbf{k})E(t,\mathbf{k})\overleftarrow{\partial}_t E^{-1}(t,\mathbf{k})B(t,\mathbf{k}). \tag{A2b}$$

Recall the form of $E(t,\mathbf{k})$ in (2.27).

In a similar manner, we can write the thermal doublet wave function $v(t,\mathbf{k})$ with the negative frequency

$$iD^-(t,\mathbf{k})^{\mu\nu}v(t,\mathbf{k})^\nu = 0, \tag{A3a}$$

$$i\bar{v}(t,\mathbf{k})^\nu \overleftarrow{D}^-(t,\mathbf{k})^{\nu\mu} = 0, \tag{A3b}$$

where

$$D^-(t,\mathbf{k}) = B^{-1}(t,\mathbf{k})E^{-1}(t,\mathbf{k})\partial_t E(t,\mathbf{k})B(t,\mathbf{k}), \tag{A4a}$$

$$\overleftarrow{D}^-(t,\mathbf{k}) = B^{-1}(t,\mathbf{k})E^{-1}(t,\mathbf{k})\overleftarrow{\partial}_t E(t,\mathbf{k})B(t,\mathbf{k}). \tag{A4b}$$

A difficulty in constructing a semifree field by making a linear superposition of $u(x,\mathbf{k})$ and $v(x,\mathbf{k})$ is due to the fact that $D^+(t,\mathbf{k})$ and $D^-(t,\mathbf{k})$ do not commute with each other when we consider a time-dependent situation. Therefore, in this Appendix, we restrict our considerations to a time-independent situation only. Then $B(t,\mathbf{k})$, $\omega(t,\mathbf{k})$, and $k(t,\mathbf{k})$ become independent of time. These quantities will be written simply as $B(\mathbf{k})$, $\omega(\mathbf{k})$, and $\kappa(\mathbf{k})$. Then according to (2.27), $E(t,\mathbf{k})$ takes the following simple form:

$$E(t,\mathbf{k}) = \exp[\,-i\{\omega(\mathbf{k}) - i\kappa(\mathbf{k})\tau_3\}t\,]. \tag{A5}$$

According to (2.33), we have

$$D^+(t,\mathbf{k}) = \partial_t + i\{\omega(\mathbf{k}) - i\kappa(\mathbf{k})A(\mathbf{k})\}, \tag{A6a}$$

$$\overleftarrow{D}^+(t,\mathbf{k}) = \overleftarrow{\partial}_t - i\{\omega(\mathbf{k}) - i\kappa(\mathbf{k})A(\mathbf{k})\}. \tag{A6b}$$

The matrix $A(\mathbf{k})$ was given in (2.38).

Similarly, we obtain

$$D^-(t,\mathbf{k}) = \partial_t - i\{\omega(\mathbf{k}) - i\kappa(\mathbf{k})A(\mathbf{k})\}, \tag{A7a}$$

$$\overleftarrow{D}^-(t,\mathbf{k}) = \overleftarrow{\partial}_t + i\{\omega(\mathbf{k}) - i\kappa(\mathbf{k})A(\mathbf{k})\}. \tag{A7b}$$

We also construct the wave functions in such a manner

that

$$u(x,\mathbf{k}) = u(t,\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}}, \tag{A8a}$$

$$\bar{u}(x,\mathbf{k}) = \bar{u}(t,\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}, \tag{A8b}$$

$$v(x,\mathbf{k}) = v(t,\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}, \tag{A9a}$$

$$\bar{v}(x,\mathbf{k}) = \bar{v}(t,\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}}. \tag{A9b}$$

Then (A1), (A3), (A6), and (A7) lead to the orthogonality condition at any time t,

$$\int d^3x\, \bar{u}(x,\mathbf{k})\Gamma v(x,\mathbf{l}) = 0, \tag{A10a}$$

$$\int d^3x\, \bar{v}(x,\mathbf{k})\Gamma u(x,\mathbf{l}) = 0, \tag{A10b}$$

where

$$\Gamma = i\overleftrightarrow{\partial_t} = i(\partial_t - \overleftarrow{\partial_t}). \tag{A11}$$

Therefore we define the inner product of two wave functions by

$$\int d^3x\, \bar{g}(x,)\Gamma f(x). \tag{A12}$$

It is obvious from (A8) and (A9) that we can choose the wave functions to satisfy

$$\int d^3x\, \bar{u}(x,\mathbf{k})\Gamma u(x,\mathbf{l}) = \rho_u \delta(\mathbf{k}-\mathbf{l}), \tag{A13a}$$

$$\int d^3x\, \bar{v}(x,\mathbf{k})\Gamma v(x,\mathbf{l}) = \rho_v \delta(\mathbf{k}-\mathbf{l}). \tag{A13b}$$

Here $\rho_u = 1$ or -1 and $\rho_v = 1$ or -1. Thus $\{u(x,\mathbf{k}), v(x,\mathbf{k})\}$ forms an orthonormalized complete set.

In order to relate u to v, we note that

$$D^+(t,\mathbf{k})^T = B^T(\mathbf{k})E^{-1}(t,\mathbf{k})\overleftarrow{\partial_t}E(t,\mathbf{k})B^{-1T}(\mathbf{k}), \tag{A14}$$

$$= B^T(\mathbf{k})B(\mathbf{k})\overleftarrow{D}^-(t,\mathbf{k})B^{-1}(\mathbf{k})B^{-1T}(\mathbf{k}), \tag{A15}$$

$$\overleftarrow{D}^+(t,\mathbf{k})^T = B^T(\mathbf{k})E^{-1}(t,\mathbf{k})\partial_t E(t,\mathbf{k})B^{-1T}(\mathbf{k}), \tag{A14'}$$

$$= B^T(\mathbf{k})B(\mathbf{k})D^-(t,\mathbf{k})B^{-1}(\mathbf{k})B^{-1T}(\mathbf{k}), \tag{A15'}$$

which follow from (A2) and (A4). Here T means the transposition. Thus (A1) leads to (A3) when we choose

$$\bar{v}(t,\mathbf{k}) = \bar{v}_0(\mathbf{k})u^T(t,\mathbf{k})B^T(\mathbf{k})B(\mathbf{k}), \tag{A16a}$$

$$v(t,\mathbf{k}) = B^{-1}(\mathbf{k})B^{-1T}(\mathbf{k})\bar{u}^T(t,\mathbf{k})v_0(\bar{k}), \tag{A16b}$$

where v_0 and $\bar{v}_0$ satisfy

$$\bar{v}_0 v_0 = 1 \tag{A16c}$$

and are arbitrary otherwise.

According to (3.4) we have

$$u(x,\mathbf{k}) = U(\mathbf{x},\mathbf{k})B^{-1}(\mathbf{k})E(t,\mathbf{k})B(\mathbf{k}), \tag{A17a}$$

$$\bar{u}(x,\mathbf{k}) = B^{-1}(\mathbf{k})E^{-1}(t,\mathbf{k})B(\mathbf{k})\bar{U}(\mathbf{x},\mathbf{k}). \tag{A17b}$$

Since the normalization condition in (A13a) differs from the one in (3.7) by the presence of Γ, we should modify the definition of $U(\mathbf{x},\mathbf{k})$ and $\bar{U}(\mathbf{x},\mathbf{k})$. Since $A(\mathbf{k})$ commutes with $D^{\pm}(t,\mathbf{k})$ according to (A6) and (A7) we choose

$$U(\mathbf{x},\mathbf{k}) = [1/(2\pi)^{3/2}]F[A(\mathbf{k})]e^{i\mathbf{k}\cdot\mathbf{x}}, \tag{A18a}$$

$$\bar{U}(\mathbf{x},\mathbf{k}) = [1/(2\pi)^{3/2}]F[A(\mathbf{k})]e^{-i\mathbf{k}\cdot\mathbf{x}}, \tag{A18b}$$

where $F[A(\mathbf{k})]$ is a function of the matrix $A(\mathbf{k})$. Equations (2.38) and (A5) show that $B^{-1}(\mathbf{k})E(t,\mathbf{k})B(\mathbf{k})$ is also a function of $A(\mathbf{k})$, implying that $A(\mathbf{k})$ commutes with $B^{-1}(\mathbf{k})E(t,\mathbf{k})B(\mathbf{k})$. Now (A16) lead to

$$v(x,\mathbf{k}) = [1/(2\pi)^{3/2}]B^{-1}(\mathbf{k})E^{-1}(t,\mathbf{k})B^{-1T}(\mathbf{k}) \times F[A^T(\mathbf{k})]v_0(\mathbf{k})e^{-i\mathbf{k}\cdot\mathbf{x}}, \tag{A19a}$$

$$\bar{v}(x,\mathbf{k}) = [1/(2\pi)^{3/2}]\bar{v}_0(\mathbf{k})F[A^T(\mathbf{k})] \times B^T(\mathbf{k})E(t,\mathbf{k})B(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{x}}. \tag{A19b}$$

Feeding (A17) with (A18) into (A13a), we obtain

$$2F^2[A(\mathbf{k})]\{\omega(\mathbf{k}) - i\kappa(\mathbf{k})A(\mathbf{k})\} = \rho_u. \tag{A20}$$

When we choose

$$\rho_u = 1, \tag{A21}$$

we have

$$F[A(\mathbf{k})] = (1/\sqrt{2})\{\omega(\mathbf{k}) - i\kappa(\mathbf{k})A(\mathbf{k})\}^{-1/2}. \tag{A22}$$

On the other hand, (A13b) together with (A19) and (A16c) gives

$$\rho_v = -2F^2[A^T(\mathbf{k})]\{\omega(\mathbf{k}) - i\kappa(\mathbf{k})A^T(\mathbf{k})\} = -1. \tag{A23}$$

We now construct the field

$$\psi(x)^\mu = \int d^3k\, [u(x,\mathbf{k})^{\mu\nu}a(\mathbf{k})^\nu + v(x,\mathbf{k})^{\mu\nu}\bar{b}^T(\mathbf{k})^\nu], \tag{A24a}$$

$$\bar{\psi}(x)^\mu = \int d^3k\, [\bar{a}(\mathbf{k})^\nu \bar{u}(x,\mathbf{k})^{\nu\mu} + b^T(\mathbf{k})^\nu \bar{v}(x,\mathbf{k})^{\nu\mu}], \tag{A24b}$$

where we introduced two sets of thermal doublet oscillators, $\{a(\mathbf{k}),\bar{a}(\mathbf{k})\}$ and $\{b(\mathbf{k}),\bar{b}(\mathbf{k})\}$. Note that the positive- and negative-frequency parts of the fields ψ^μ and $\bar{\psi}^\mu$ are transformed separately under the tilde operation (2.4) if v_0 and $\bar{v}_0$ in (A16) are kept arbitrary. Therefore we choose v_0 and $\bar{v}_0$ as

$$v_0(\mathbf{k}) = \bar{v}_0(\mathbf{k}) = B^T(\mathbf{k})\tau_3 B(\mathbf{k}), \tag{A25}$$

so that ψ^μ and $\bar{\psi}^\mu$ have the definite transformation property of the tilde conjugation:

$$[\psi(x)^1]^\sim = -\bar{\psi}(x)^2, \tag{A26a}$$

$$[\psi(x)^2]^\sim = \bar{\psi}(x)^1, \tag{A26b}$$

$$[\bar{\psi}(x)^1]^\sim = \psi(x)^2, \tag{A26c}$$

$$[\bar{\psi}(x)^2]^\sim = -\psi(x)^1. \tag{A26d}$$

The semifree field equations are

$$D^+(t,-i\nabla)D^-(t,-i\nabla)\psi(x) = 0, \tag{A27a}$$

$$\bar{\psi}(x)\overleftarrow{D}^-(t,i\overleftarrow{\nabla})\overleftarrow{D}^+(t,i\overleftarrow{\nabla}) = 0, \tag{A27b}$$

which read as

$$[\partial_t^2 + \{\omega(-i\nabla) - i\kappa(-i\nabla)A(-i\nabla)\}^2]^{\mu\nu}\psi(x)^\nu = 0, \tag{A28a}$$

$$\bar{\psi}(x)^\nu[\overleftarrow{\partial}_t^2 + \{\omega(i\overleftarrow{\nabla}) - i\kappa(i\overleftarrow{\nabla})A(i\overleftarrow{\nabla})\}^2]^{\nu\mu} = 0. \tag{A28b}$$

These equations of motion can be derived from the Lagrangian density

$$\hat{L}^0 = -\bar{\psi}(x)^\mu[\partial_t^2 + \{\omega(-i\nabla) - i\kappa(-i\nabla)A(-i\nabla)\}^2]^{\mu\nu}\psi(x)^\nu. \tag{A29}$$

This gives the canonical conjugate momentum field of ψ as

$$\bar{\pi} = \frac{\partial}{\partial t}\bar{\psi}. \tag{A30}$$

We can easily derive the following sum rules:

$$i\Delta^+(x-x')^{\mu\nu} = \int d^3k\, u(x,\mathbf{k})^{\mu\lambda}\bar{u}(x',\mathbf{k})^{\lambda\nu}, \tag{A31a}$$

$$i\Delta^-(x-x')^{\mu\nu} = -\int d^3k\, v(x,\mathbf{k})^{\mu\lambda}\bar{v}(x',\mathbf{k})^{\lambda\nu}, \tag{A31b}$$

where

$$\Delta^{\pm}(x) = \mp i\int \frac{d^3k}{(2\pi)^3} \times \frac{\exp[\mp i\{\omega(\mathbf{k}) - i\kappa(\mathbf{k})A(\mathbf{k})\}t]\exp[\pm i\mathbf{k}\cdot\mathbf{x}]}{2\{\omega(\mathbf{k}) - \kappa(\mathbf{k})A(\mathbf{k})\}}. \tag{A32}$$

The functions $\Delta^{\pm}$ have the following properties:

$$\Delta^+(-x) = -\Delta^-(x), \tag{A33a}$$

$$\delta(t)\frac{\partial}{\partial t}\Delta^{\pm}(x) = -\frac{1}{2}\delta(\mathbf{x})\delta(t), \tag{A33b}$$

$$[\partial_t^2 + \{\omega(-i\nabla) - i\kappa(-i\nabla)A(-i\nabla)\}^2]\Delta^{\pm}(x) = 0. \tag{A33c}$$

The sum rules (A31) lead to the commutation relation

$$[\psi(x)^{\mu},\bar{\psi}(x')^{\nu}] = i\Delta(x-x')^{\mu\nu}, \tag{A34}$$

where

$$\Delta(x) \equiv \Delta^+(x) + \Delta^-(x). \tag{A35}$$

We call (A31) the canonical sum rules, since (A33b), (A34), (A30), and (A24) give the equal-time canonical commutation relation

$$[\psi(x)^{\mu},\bar{\pi}(x')^{\nu}]\delta(t-t') = i\delta^{\mu\nu}\delta^{(4)}(x-x'). \tag{A36}$$

Thus we have explicitly constructed the canonical formalism for the semifree field of type 2 in the time-independent thermal situation. Note that the parameter b_R was never fixed in this formulation. This freedom includes the freedom in choice of the α parameter which was discussed in several previous papers.[4,7] We have not succeeded in extending this formulation of type 2 semifree fields to a time-dependent situation.

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There is no isolated *p-p* wave

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A theorem is presented that basically states that there are no nontrivial well-behaved, spatially asymptotically flat space-times which are *p-p* waves at infinity.

I. INTRODUCTION

Space-times with a constant null vector (*p-p* waves) have been studied extensively in the literature.[1] Almost always, these space-times are interpreted physically as infinite plane gravitational waves. There are, however, attempts to construct *p-p* waves to represent, instead of waves, particles moving at the speed of light.[2,3] But any notion of isolated particles would naturally restrict the space-times under consideration to the class of spatially asymptotically flat space-times. Of all the solutions proposed, only one[3] is clearly spatially asymptotically flat (this solution is also vacuum and axisymmetric). Perhaps, the most intriguing aspect of the solution is that it has a vanishing ADM momentum, and yet it is not flat. On closer examination, we see that it gets around the positive mass theorem[4,5] because it does not have a complete spacelike surface. A natural question thus arises: can one construct a *p-p* wave that is well behaved (spatially complete) and spatially asymptotically flat? In this paper, we present a theorem which basically states that a spatially complete space-time satisfying the dominant energy condition and that is a *p-p* wave at least at infinity cannot be asymptotically flat unless it is flat. Thus we see that no well-behaved space-times based on the *p-p* waves can be constructed to represent an isolated particle.

In Sec. II we will briefly look at the solution proposed in Ref. 3. Section III contains the precise statement and the proof of the theorem mentioned above.

II. A METRICAL SOLITON

The space-time (M,g_{ab}) of interest reported in Ref. 3, representing a "metrical soliton," has the metric in the following form:

$$ds^2 = \frac{\rho^2}{\rho^2+\chi}d\rho^2 + (\rho^2+\chi)d\psi^2 + \left[1 - \frac{(\partial\chi/\partial z)^2}{4(\rho^2+\chi)}\right]dz^2 - \left[1 + \frac{(\partial\chi/\partial z)^2}{4(\rho^2+\chi)}\right](dx^4)^2 - \frac{1}{2}\frac{\alpha(\partial\chi/\partial z)^2}{(\rho^2+\chi)}dz\,dx^4, \tag{1}$$

where (ρ,ψ,z,x^4) are the standard cylindrical coordinates. Here χ is a compact supported function of $(z+\alpha t)$, with $\alpha = \pm 1$. The basic facts concerning this metric (axisymmetric, *p-p* wave) can be easily verified. Of special interest is that the space-time admits a spatially asymptotically flat hypersurface Σ. In fact, the desired surface is given by $x^4 = 0$.

To see this more clearly, introduce on $\Sigma = \{x^4 = 0\}$ the usual rectangular coordinates (x,y,z) with $x = \rho\cos\psi$, $y = \rho\sin\psi$. Then on Σ the components of the first and second fundamental forms, h_{ij} and π_{ij}, respectively, in the rectangular coordinates, have the following asymptotic properties:

$$h_{ij} = \delta_{ij} + O(1/r^2), \quad \pi_{ij} = O(1/r^3).$$

Thus Σ is asymptotically flat. Moreover, since the fall-offs are one power of $1/r$ faster than the standard ones, the ADM four-momentum of M on Σ has to vanish.

To understand how the space-time can be reconciled with the positive mass theorem, it suffices to examine the induced metric h_{ij} on Σ. It has the form, in the (ρ,ψ,z) coordinates,

$$\text{spatial metric} = \left(\frac{\rho^2}{\rho^2+\chi}\right)d\rho^2 + (\rho^2+\chi)d\psi^2 + \left[1 - \frac{(\partial\chi/\partial z)^2}{4(\rho^2+\chi)}\right]dz^2.$$

To ensure that Σ is spacelike, the conditions $\chi \geqslant 0$ and $4(\rho^2+\chi) \geqslant (\partial x/\partial z)^2$ must hold. Even with these provisions, the spatial metric is degenerate at the line $\rho = 0$, unless $\chi \equiv 0$, in which case the space-time metric is flat. To remove this irregularity, one can, for example, cut out the line $\rho = 0$ from Σ. But then Σ will be incomplete. In conclusion, it is obvious that the only well-behaved (nondegenerate and complete) space-time metric of the form (1) is flat.

III. THERE IS NO ISOLATED *p-p* WAVE

Of course it would be tempting to patch up the metric (1) so that it becomes complete and still retains the *p-p* wave nature of the solution. However, any attempt in this direction, without violating the dominant energy condition, would be unsuccessful. The following theorem elucidates this situation.

Theorem: Let (M,g_{ab}) be a spatially asymptotically flat space-time with Σ as an asymptotically flat spacelike complete surface. Suppose (a) there exists a covariantly constant null vector k^a in a neighborhood of $(\Sigma - K)$, where K is a compact set of Σ, and (b) the dominant energy condition holds on Σ; then (M,g_{ab}) is flat along Σ.

The proof of the theorem follows easily from the following two lemmas. The conditions in the theorem are assumed in the following discussion.

Lemma: There exists a covariant constant spinor ξ^A in a neighborhood of $(\Sigma - B)$, where B is a compact set of Σ.

Proof: Consider the covariant null vector k^a, in the

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theorem. Anticommuting second derivatives of k^a leads to $R_{abcd}k^d = 0$, and by contracting, $R_{ad}k^d = 0$. The dominant energy condition further implies that $R_{ab} = fk_a k_b$ for some f. Finally, it is easy to conclude that $C_{abcd}k^d = 0$.

Now, let ξ^A be the spinor such that $\xi^A \bar{\xi}^{A'} = k^a$. Here $\nabla_a k_b = 0$ implies (in a neighborhood of $\Sigma - K$) that

$$\nabla_a \xi_B = iv_a \xi_B,$$

where v_a is a real vector field. Anticommuting second derivatives gives

$$\nabla_{[a}\nabla_{b]}\xi_C = i\nabla_{[a}v_{b]}\xi_C.$$

The left-hand side of the above equation actually vanishes. To see this, consider the standard spinor representation of the curvature tensors (see, e.g., Ref. 6),

$$C_{abcd} = \psi_{ABCD}\epsilon_{A'B'}\epsilon_{C'D'} + \text{c.c.},$$

$$R_{ab} = -2\Phi_{A'B'AB} + 6\Lambda\epsilon_{A'B'}\epsilon_{AB},$$

and

$$R = -24\Lambda.$$

Then

$$\nabla_{[a}\nabla_{b]}\xi_C = \psi^D_{ABC}\epsilon_{A'B'}\xi_D + \Phi^D_{A'B'C}\epsilon_{AB}\xi_D + \Lambda(\epsilon_{AC}\epsilon^D_B + \epsilon_{BC}\epsilon^D_A)\epsilon_{A'D'}\xi_D.$$

Since $C_{abcd}k^a = 0$ and $R_{ab} = fk_a k_b$, the right-hand side of the above equation vanishes. Thus

$$\nabla_{[a}v_{b]} = 0.$$

Now take a compact set $B(\supseteq K)$ of Σ such that $\Sigma - B$ is simply connected (for instance, take B to be the coordinate R ball, B_R for R sufficiently large). Therefore, $v_b = \nabla_b g$, for some g in $\Sigma - B$. Finally, the following rephasing of ξ^A: $\xi^A \to \exp(-ig)\xi^A$, yields $\nabla_a \xi_B = 0$ in $\Sigma - B$. Q.E.D.

The following definition (see also Refs. 5, 7, and 8) is relevant for the second lemma.

Definition: A spinor field ξ^A on $\Sigma - B$, where B is a compact set of Σ, is called asymptotically constant if

$$\xi^A \underset{r\to\infty}{\to} \overset{0}{\xi}{}^A + O(1/r),$$

where r is the asymptotically flat radial coordinate of Σ, and $\overset{0}{\xi}{}^A$ is a constant spinor as defined by a tetrad associated with the asymptotically flat coordinates on Σ.

Lemma: A covariantly constant spinor is asymptotically constant.

Proof: Introduce a norm (see, e.g., Ref. 9) on the spinors by $\langle \xi^A, \eta_A \rangle = \xi^A \eta^{A'} t_{AA'}$, where $t_{AA'}$ is the unit normal to Σ. Choose two constant spinors $\overset{0}{\xi}{}^A$ and $\overset{0}{\eta}{}^A$ at infinity such that $\overset{0}{\xi}{}^A \overset{0}{\eta}{}_A = 1$, and they are orthonormal with respect to $\langle\ ,\ \rangle$. Now

$$\xi^A = \alpha \overset{0}{\xi}{}^A + \beta \overset{0}{\eta}{}^A, \quad \text{for some } \alpha \text{ and } \beta.$$

For ξ^A to be asymptotically constant, α and β should have the correct asymptotic properties, namely, $\alpha \to_{r\to\infty} \alpha_0 + O(1/r)$ and $\beta \to_{r\to\infty} \beta_0 + O(1/r)$, with α_0 and β_0 constant. We will first establish that the norm

$$|\xi^A| = \langle \xi^A, \xi^A \rangle^{1/2} = (\bar{\alpha}\alpha + \bar{\beta}\beta)^{1/2}$$

has the right asymptotic properties.

Taking a derivative and noting that $\nabla_a \xi^A = 0$, give

$$\nabla_b |\xi^A|^2 = \xi^A \bar{\xi}^{A'} \nabla_b t_a.$$

Projecting by h^c_b, we obtain

$$D_b |\xi^A|^2 = s^a \pi_{ba},$$

with $s^a = h^a_b k^b$. Now let v^b be any unit vector of Σ (with respect to h_{ab}); then

$$v^b D_b |\xi^A|^2 = s^a v^b \pi_{ba},$$

$$|v^b D_b |\xi^A|\,| = |s_c h^{cd} v^b \pi_{bd}| \leqslant |s^a|\,|v^b \pi_b{}^d|,$$

where $|m^a|$, for instance, is $(-h_{ab}m^a m^b)^{1/2}$ for any m^a on Σ. [Note that since the space-time metric has signature $(+,-,-,-)$ in accordance with the spinor convention h_{ab}, the induced metric on Σ is negative definite; hence the negative sign in the above inner product for vectors on Σ.] Now

$$k^a k_a = \xi^A \bar{\xi}^{A'} g_{ab} \xi^B \bar{\xi}^{B'} = \xi^{AA'}(h_{ab} + t_a t_b)\xi^A \bar{\xi}^{B'} = -|s^a|^2 + |\xi^A|^4.$$

Since k^a is null,

$$|x^a| = |\xi^A|^2.$$

Thus

$$|v^b D_b |\xi^A|^2| \leqslant |\xi^A|^2 |v\pi^a|.$$

By the assumption of asymptotic flatness, $|v^a \pi_a{}^b| = O(1/r^2)$. Therefore, there exists positive constants C and r_0 such that

$$|v^b D_b \ln|\xi^A|\,| \leqslant C/r^2 \quad \text{for } r \geqslant r_0. \tag{2}$$

Now, suppose $v^b = r^a$, the vector $(\partial/\partial r)^a$. Though r^a is not strictly a unit vector, its norm differs from unity only by terms of order $(1/r)$ and higher. Therefore we can still use the above inequality, which yields

$$\left| \frac{\partial}{\partial r} \ln|\xi^A| \right| \leqslant \frac{C}{r^2}.$$

Upon integration, the above gives

$$C/r - C/r_0 \leqslant \ln|\xi^A(r,\theta,\phi)| - \ln|\xi^A(r_0,\theta,\phi)| \leqslant C/r_0 - C/r.$$

It is then clear that $\lim_{r\to\infty} \ln|\xi^A(r,\theta,\phi)|$ exists. Let

$$\lim_{r\to\infty} \ln|\xi^A(r,\theta,\phi)| = \ln N(\theta,\phi),$$

which implies $\lim_{r\to\infty} |\xi^A(r,\theta,\phi)| = N(\theta,\phi)$. The above inequality further asserts

$$|\xi^A(r,\theta,\phi)| \underset{r\to\infty}{\to} N(\theta,\phi) + O(1/r).$$

The following argument establishes that $N(\theta,\phi)$ is, in fact, independent of θ and ϕ. Define $M(r) > 0$ such that

$$\ln M(r) = \frac{1}{4\pi}\int \ln|\xi^A(r,\theta,\phi)| \sin\theta\, d\theta\, d\phi.$$

Now,

$$\max|\ln M(r) - \ln|\xi^A(r,\theta,\phi)|\,|$$
$$\leqslant C' r \max|v^a D_a \ln|\xi^A(r,\theta,\phi)|\,|,$$

where C' is a positive constant and v^a is any unit vector on the sphere S_r; and

$$\max|\ln M(r) - \ln|\xi^A(r,\theta,\phi)|\,| \leqslant C''/r,$$

where C'' is a positive constant. Consequently for sufficiently large r,

$$\max|\ln M(r) - \ln N(\theta,\phi)| \leqslant C'''/r,$$

C''' is a positive constant.

Now it is obvious that $N(\theta,\phi)$ is independent of (θ,ϕ) up to order $1/r$. Finally we conclude that

$$|\xi^A(r,\theta,\phi)| \underset{r\to\infty}{\to} N + O(1/r),$$

where N is a constant.

Similar considerations lead to the desired results $\alpha \to_{r\to\infty} \alpha_0 + O(1/r)$, and $\beta \to_{r\to\infty} \beta_0 + O(1/r)$. Q.E.D.

The previous two lemmas can now be employed to establish the theorem. Consider the following integral:

$$S = \int_{S^2} ds^a\, t_b \eta^B \nabla_a \eta^{B'},$$

with ds^a the surface element of S^2, a sphere at infinity, t^a the unit normal to Σ, and η^A a spinor. If η^A is an asymptotically constant spinor satisfying the Witten equation, $D_{AA'}\eta^{A'} = 0$, where $D_a = h_{ab}\nabla_b$, then[5,7]

$$S = \kappa P^a_{\mathrm{ADM}} \underset{0}{\eta}_A \underset{0}{\eta}_{A'},$$

P^a_{ADM} is the ADM four-momentum of (M, g_{ab}) along Σ, $\underset{0}{\eta}^A$ is the constant spinor to which η_A approaches, and κ is a constant. But by the previous lemmas, there exists outside a compact set of Σ, a covariantly constant spinor ξ^A (thus satisfying the Witten equation), which is also an asymptotically constant spinor. Here S must vanish for this spinor ξ^A, and thus

$$P^a_{\mathrm{ADM}} \underset{0}{\xi}_A \underset{0}{\xi}_{A'} = 0.$$

But since P^a_{ADM} is strictly timelike,[10,11] it therefore vanishes. In conclusion, by the positive mass theorem, (M, g_{ab}) is flat along Σ. Q.E.D.

IV. CONCLUSION

Thus we have shown that a truly well-behaved isolated object which is a p-p wave at infinity cannot exist. We would like to point out in closing that if one were to relax any of the conditions in the theorem, one could easily obtain p-p waves which are spatially asymptotically flat.[3] Thus the conditions in the theorem are the weakest one can assume for the theorem to hold.

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Some solutions of Einstein's equations with shock waves

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The Einstein field equations in the presence of a polytropic fluid performing self-similar motion are reduced to a dynamical system. Qualitative properties of the dynamical system are investigated in the case when the fluid motion is with shock waves.

I. INTRODUCTION

Solutions of Einstein's equations with shock waves can be relevant in several areas of astrophysics. In particular, relativistic fluid motions with shocks occur in (1) nonlinear evolution of an initial adiabatic perturbation in the radiation dominated phase of the universe (in the standard scenario, neglecting the presence of collisionless particles)[1]; (2) nonlinear collapse of an adiabatic perturbation in the matter dominated phase[1]; (3) explosions in the intergalactic medium and hydrodynamical models of galaxy formation[2]; and (4) bubble growth in the phase transition assumed to occur in some models of the early universe.[3]

The problem of the evolution of cosmic thin shells has been tackled by using a general relativistic numerical code by Sato and co-workers.[4–6] A thin shell is to be distinguished from a shock wave, because in the former there is a source of energy-momentum within the surface layer (and this is modeled as a δ-function discontinuity in the energy-momentum tensor). Thin shells could be reasonable models for propagating detonation waves.

Here we shall limit ourselves to shock waves which correspond to the approximation of neglecting the source of energy-momentum within the surface layer compared to the total explosion energy.

Cases (3) and (4) have been investigated by looking for similarity solutions in the framework of Newtonian fluid dynamics[2,7,8] and special relativistic fluid dynamics, respectively.[3]

From the mathematical point of view it is very difficult to study general relativistic fluid motion without any symmetry. Therefore we choose to work in spherical symmetry (which is a very good approximation in the case when the source of the motion can be considered a point explosion). Even with this limitation the resulting equations are partial differential equations (PDE's) and a full analysis is still very difficult and in general one has PDE's to resort to numerical calculations.

In order to obtain a mathematically tractable problem we restrict ourselves to self-similar motion (which should be a good approximation asymptotically far from the source) and in this way the system of PDE's is reduced to a dynamical system to which we can apply the qualitative theory.[9] In a previous paper[10] one of us talked about the problem of the behavior of a self-similar shock wave in an expanding universe in the case of a barotropic fluid. In the present paper, among other things we also provide analytical proofs of some features of the fluid motion which were discovered by numerical integration.

The plane of the paper is the following: In Sec. II the basic equations in the case of a polytropic state equation are derived. In Sec. III the barotropic fluid case is revisited and a Lyapunov function for the dynamical system is found. In Sec. IV qualitative properties of the expanding self-similar shock wave in a barotropic fluid are studied. In Sec. V configurations with two expanding shock waves are analyzed. In Sec. VI some qualitative properties of the dynamical system in the politropic case are discussed. In Sec. VII still in the polytropic case a numerical integration is performed for an expanding shock wave in a Friedmann dust universe.

II. BASIC EQUATIONS

In Ref. 11 it is shown that the most general self-similar spherically symmetric space-time, in a fluid comoving reference frame, is

$$ds^2 = e^{2\varphi(z)}\,dt^2 - e^{2\psi(z)}\,dR^2 - R^2\mathscr{R}^2(z)d\Omega^2,$$
$$d\Omega^2 = d\theta^2 + \sin^2\theta\,d\chi^2, \tag{1}$$

where $z = R/t$, the fluid velocity is $U^a = (e^{-\varphi},0,0,0)$ and the vector $V^a = (t,R,0,0)$ is a homothetic Killing vector, that is, $L_V g_{ab} = 2g_{ab}$, where L_V is the Lie derivative along V.

In a reference frame adapted to the vector field V the metric (1) takes the following conformally static form[9]:

$$ds^2 = e^{2\tau}(e^{\nu(r)}\,d\tau^2 - e^{\lambda(r)}\,dr^2 - r^2\,d\Omega^2), \tag{2}$$

and the vector fields U and V become, respectively,

$$U^a = (e^{-\tau-\nu/2}/\sqrt{1-u^2},$$
$$ue^{-\tau-\lambda/2}/\sqrt{1-u^2},\ 0,\ 0), \tag{3}$$
$$V^a = (1,0,0,0). \tag{4}$$

where $u = u(r)$ is the spatial velocity of the fluid with respect to the hypersurfaces $r = \text{const}$.

In the following, the energy momentum tensor of a perfect fluid will be considered, that is,

$$T_{ab} = (p+\epsilon)U_a U_b - pg_{ab}, \tag{5}$$

where p and ϵ denote, respectively, the pressure and the total energy density, which by self-similarity have the following form:

$$p(\tau,r) = e^{-2\tau}\bar{p}(r), \quad \epsilon(\tau,r) = e^{-2\tau}\bar{\epsilon}(r). \tag{6}$$

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Furthermore, it will be assumed the state equation

$$p=(\gamma-1)(\epsilon-c\rho), \tag{7}$$

where $\rho(\tau,r)=e^{-2\tau}\bar{\rho}(r)$ is the total density of matter, and γ and c are constants such that $1<\gamma<2$ and $c=0$ or $c=1$. In the first case Eq. (6) is the barotropic state equation and in the last one is the polytropic state equation.

In both cases the sound velocity a is given by

$$a^2=\gamma p/(p+\epsilon). \tag{8}$$

From Eqs. (7) and (8) it follows that

$$\bar{\epsilon}=(\gamma-a^2)(\bar{p}+\bar{\epsilon})/\gamma, \tag{9}$$

$$\bar{p}=a^2(\bar{p}+\bar{\epsilon})/\gamma, \tag{10}$$

and if $c=1$,

$$\bar{\rho}=(\gamma-1-a^2)(\bar{p}+\bar{\epsilon})/(\gamma-1). \tag{11}$$

By letting $z=\ln r$, $\dot{}=d/dz$, $Q=re^{(\lambda-\nu)/2}$, $w=\dot{\nu}=r\,d\nu/dr$, Einstein's equations $R^0{}_0-R^1{}_1=\varkappa(T^0{}_0-T^1{}_1)$, $R^2{}_2-\frac{1}{2}R=\varkappa T^2{}_2$, the energy-momentum conservation laws $T^a{}_{0;a}=0$, $T^a{}_{1;a}=0$, and the baryon number conservation law $(\rho U^a)_{;a}=0$ give the following evolution equations:

$$\dot{Q}=Q(1-w-Q^2-wQ(1+u^2)/(2u)), \tag{12}$$

$$\dot{w}=-w(1+w+Q^2-(Q/u)((1+(w/2))(1+u^2)+(2a^2/\gamma)(1-u^2))), \tag{13}$$

$$\dot{u}=-(1-u^2)(Q(u^2-3a^2+2(a^2/\gamma)(1-u^2))+(w/2)u(1-a^2)-2ua^2)/(u^2-a^2), \tag{14}$$

$$\dot{a}=a(\gamma-1-a^2)((w/4)(1-u^2)-u^2-(Q/u)\times(u^2-(a^2/\gamma)(1-u^2)))/(u^2-a^2). \tag{15}$$

By letting $L=e^{\lambda}$, Einstein's equation $R^1{}_1-\frac{1}{2}R=\varkappa T^1{}_1$, gives the constraint equation

$$L=1+w-Q^2+(wQ/u)(u^2+(a^2/\gamma)(1-u^2))>0, \tag{16}$$

and the equation $R_{01}=\mathscr{L}T_{01}$ gives

$$\bar{p}+\bar{\epsilon}=-wQ(1-u^2)/(\varkappa r^2uL). \tag{17}$$

From Eqs. (9)–(11) and (17) one obtains the functions $\bar{p}$, $\bar{\epsilon}$, $\bar{\rho}$ when a solution of the dynamical system (12)–(15) is known. Furthermore, Eq. (17) gives the constraint

$$\operatorname{sgn}(u)=-\operatorname{sgn}(w). \tag{18}$$

The mass conservation law $(\rho U^a)_{;a}=0$ may be written in the following form:

$$(\dot{\bar{\rho}}/\bar{\rho})+(Q/u)+(w/2)+2+\dot{u}/(u(1-u^2))=0. \tag{19}$$

By deriving the expression for $\bar{\rho}$ which follows from Eqs. (11) and (17), one obtains

$$w=-(\dot{\bar{\rho}}/\bar{\rho})+(\dot{w}/w)-(\dot{Q}/Q)-2a\dot{a}/(\gamma-1-a^2)-(1+u^2)\dot{u}/(u(1-u^2)), \tag{20}$$

and by Eqs. (14) and (15)

$$\dot{u}/(u(1-u^2))+2\dot{a}/(a(\gamma-1-a^2))=-2-(w/2)-3(Q/u). \tag{21}$$

From Eqs. (19)–(21) one obtains

$$4+2(\dot{\bar{\rho}}/\bar{\rho})-(\dot{Q}/Q)+(\dot{u}/u)+(\dot{w}/w)-2(1+a^2)\dot{a}/(a(\gamma-1-a^2)), \tag{22}$$

which gives the following first integral:

$$Qw^3a^{-2/(\gamma-1)}(1-u^2)^2(\gamma-1-a^2)^{(3\gamma-2)/(\gamma-1)}/(uL^2)=c_1<0, \tag{23}$$

where c_1 is an integration constant.

The invariant manifold $a^2=\gamma-1$ ($c_1=0$) corresponds to the barotropic case. On this invariant manifold equation (15) is identically satisfied and the dynamical system becomes[9]

$$\dot{Q}=Q(1-w-Q^2-wQ(1+u^2)/(2u)), \tag{12'}$$

$$\dot{w}=-w(1+w+Q^2-(Q/u)((1+(w/2))(1+u^2)+2k(1-u^2)/(1+k))), \tag{13'}$$

$$\dot{u}=-(1-u^2)((1-k)u(w/2)-2ku+Q\times(u^2(1-k)-k(1+3k))/(1+k))/(u^2-k), \tag{14'}$$

with the constraint equations

$$L=1+w-Q^2+wQ(k+u^2)/(u(1+k))>0, \tag{16'}$$

$$\bar{\epsilon}=-wQ(1-u^2)/(\varkappa(1+k)ur^2L), \tag{17'}$$

$$\operatorname{sgn}(u)=-\operatorname{sgn}(w), \tag{18'}$$

where $k=\gamma-1$.

III. COMMENTS ON THE BAROTROPIC CASE

The qualitative features of the dynamical system in the barotropic case has been studied extensively in Ref. 9. Here, after an outline of the behavior of the solutions, we prove a new result. The main features of the dynamical system in the region $u<0$ are pictured in Fig. 1 (in the region $u>0$ there are no physical solutions because they cannot be continued until the center even if a discontinuity is introduced).

There are two kinds of solutions in the subsonic region ($-\sqrt{k}<u<0$): solutions which cross the plane $u=-\sqrt{k}$ in a point of the line I, and solutions which arrive in the region L^r of the plane $u=-\sqrt{k}$. These latter solutions cannot be continued in the supersonic region ($u<-\sqrt{k}$) because on L^r the dynamical system change direction; the only way to continue these solutions is to join them across a discontinuity (shock wave) to a solution in the supersonic region.

We recall that a shock wave is a timelike discontinuity hypersurface such that the first and second fundamental forms are continuous and such that the following continuity conditions hold true:

$$[T^a{}_bN^b]=0, \quad [\rho U^aN_a]=0, \tag{24}$$

where the brackets indicate the jump across the discontinuity. The continuity of the first and second fundamental form is equivalent to the continuity of the variables Q, w, and L, and these latter together with Eq. (16') give the following jump conditions[9,10]:

$$[Q]=[w]=[(k+u^2)/(u(1+k))]=0. \tag{25}$$

The first of Eqs. (24) does not give further constraints, and

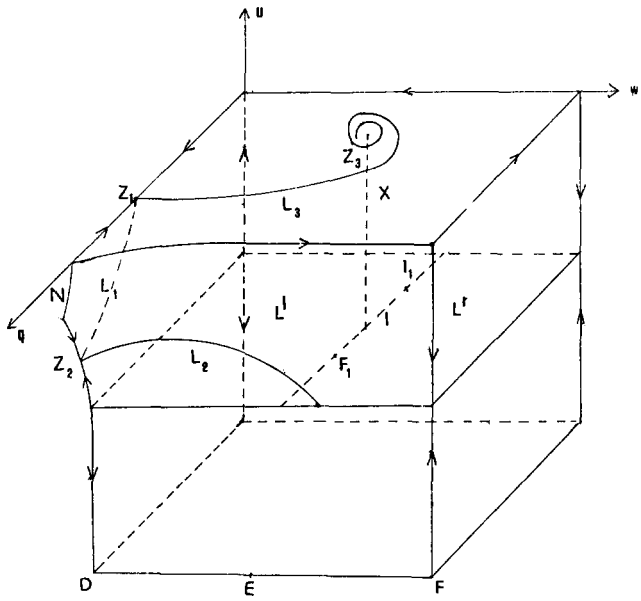

FIG. 1. Phase space of the dynamical system (12')–(14') (barotropic state equation).

the second is an identity in the barotropic case.

In the subsonic region the solutions in the interior of phase space which start from some singular point are the following.

(a) Solutions filling the two-dimensional separatrix Z of the singular point Z_1 (it is possible to identify the separatrix Z in Fig. 1 by taking into account that it intersects the component of the boundary $u=0$, $w=0$, and $L=0$, respectively, in the line L_1, L_2, and L_3).

(b) The limit line X of the separatrix Z which starts from the singular point Z_3 and corresponds to the Oppenheimer–Volkov solution. All other trajectories come from the unphysical region $u>0$ across the line N ($u=w=0$, $Q>0$).

The behavior of the latter solutions has been studied in Ref. 10 and it has been proved that it is necessary to join them across a discontinuity at $u=0$ to some solution of the full spherically symmetric Einstein equations and if this latter solution contains the center of symmetry it must possess a trapped surface and therefore a space-time singularity.

However, it is possible to avoid the singularity by making a change in the topology of solution in such way that the center of symmetry does not belong to the space-time. A trivial example in which this last solution may be realized is obtained by stopping the self-similar solution at $u=0$ and then by continuing it with its mirror image.

The qualitative behavior of the solution obtained in Ref. 9 is based on the assumption that all solutions start (end) from (to) some singular point or from the characteristic plane $u=-\sqrt{k}$, that is, it is assumed that there are no compact invariant manifolds near which solutions wind around.

Now we shall prove that there are no invariant compact manifolds. Because on a compact manifold any continuous function has a maximum, to prove the statement it is sufficient to show the existence of a Lyapunov function, that is a C^1 function $F(Q,w,u)$ defined in the interior of the dynamical system which is increasing on the solutions of Eqs. (12')–(14').

By Eqs. (12'), (13'), (14'), and (16'),

$$\dot{L} = -L(w+2Q^2+wQ(1+u^2)/u). \tag{26}$$

By deriving the function

$$F = L^{1-k}Q^{-1-k}w^{3k-1}u^{-2k}(1-u^2)^{k-1} > 0 \tag{27}$$

and by using Eqs. (12'), (13'), (14'), and (26), one obtains

$$\dot{F} = (1-k)(1+3k)FQ(1-u^2)/(u(1+k)), \tag{28}$$

which is always positive in the region $u>0$ and negative in the region $u<0$. Therefore, Eq. (27) gives a Lyapunov function in the regions $u>0$ and $u<0$ separately.

In particular, if $k=1$ one obtains the first integral

$$w/(Qu) = c_2 < 0. \tag{29}$$

IV. EXPANDING SELF-SIMILAR SHOCK WAVE IN THE FLAT FRIEDMANN UNIVERSE (BAROTROPIC CASE)

The exact solution F of the dynamical system (12')–(14') corresponding to the flat Friedmann solution has the form[9]

$$\begin{aligned} &Q = u/(\bar{\beta}-1-\bar{\beta}u^2),\\ &w = -2\bar{\beta}u^2/(\bar{\beta}-1-\bar{\beta}u^2),\\ &u = (\bar{\beta}-1)\mu,\\ &r(\mu) = C_2\mu(1-(\bar{\beta}-1)^2\mu^2)^{1/(2\bar{\beta}-2)},\\ &\bar{\beta} = 2/(3(1+k)). \end{aligned} \tag{30}$$

This solution belongs to the separatrix Z and crosses the plane L of nonextensibility of solutions ($u=-\sqrt{k}$) in a point F_1 of the line of singular points I.

Proposition 1: The intersection of the separatrix Z with the plane L in the neighborhood of the point F_1 at $0<k<\frac{1}{3}$ coincides with a segment on the line I.

Proof: In coordinates α,β, and parameter τ_1 such that

$$\begin{aligned} &\alpha = \frac{1}{Q}, \quad \beta = \frac{(1-k)w}{2Q} - \frac{2k}{Q},\\ &\frac{d\tau_1}{dz} = -\frac{Q}{u^2-k}, \end{aligned} \tag{31}$$

the eigenvalues of singular points of the segment I are[9]

$$\begin{aligned} &\lambda_{\pm} = \sqrt{k}(1-k)(-1+(1\pm 2Z_0(1-k)^{-1})^{1/2}),\\ &\lambda_3 = 0, \end{aligned} \tag{32}$$

with

$$\begin{aligned} Z_0 = {} & (2k(1+3k)/(1-k))\alpha^2 - (2\sqrt{k}/(1-k^2))\\ & \times((1+k)^3+2k(3+k^2))\alpha + 6k\\ & + 16k^2(1+k^2)/((1-k)(1+k)^2). \end{aligned}$$

After substituting in Eqs. (32) the value of parameter $\alpha = (1+5k)/(3\sqrt{k}(1+k))$, corresponding to the singular point F_1, one obtains, in the case $0<k<\frac{1}{3}$, the formulas

$$\begin{aligned} &\lambda_+ = -2\sqrt{k}(1+3k)(1-k)/(3(1+k)),\\ &\lambda_- = -4\sqrt{k}(1-k)/(3(1+k)). \end{aligned} \tag{33}$$

The corresponding eigenvectors are

$$V_+ = (1/3k, -4/(3(1+k)),1),$$
$$V_- = ((1+3k)/6k, -2(1+3k)/(3(1+k)),1). \quad (34)$$

From the formula (33) we have $\lambda_+ > \lambda_-$, so the qualitative behavior of the dynamical system near the singular point F_1 is like in Fig. 2, where L_+ and L_- denote the invariant manifolds filled by the separatrix of the singular points of the segment I.

By calculating the tangent to the trajectory F in the point F_1 it is easily seen that F corresponds to the eigenvalue λ_+, so the trajectory F is tangent to the stable two-dimensional invariant manifold L_+ filled with the separatrices of singular points of the line I corresponding to the greatest eigenvalues λ_+.

Therefore all trajectories on the two-dimensional separatrix Z, which are close to the trajectory F, are tangent to the invariant manifold L_+. Hence all of them enter a segment I_Z of the line I in a neighborhood of the point F_1. This proves the statement.

In the following we consider self-similar solutions with an expanding shock wave such that in front of the shock wave there is the Friedmann solution with state equation $p = k_1\epsilon$ and inside there is the solution, with state equation $p = k_2\epsilon$ $(k_1 < k_2 < \frac{1}{3})$, corresponding to the initial data determined by Eqs. (25).

The initial data are not uniquely determined but depend on the radial velocity $-u_2$ of the shock wave which respect to the interior fluid. Therefore there is a line G in the phase space such that the solutions defined previously (but with different Mach numbers) arrive at different points of G before the jump.

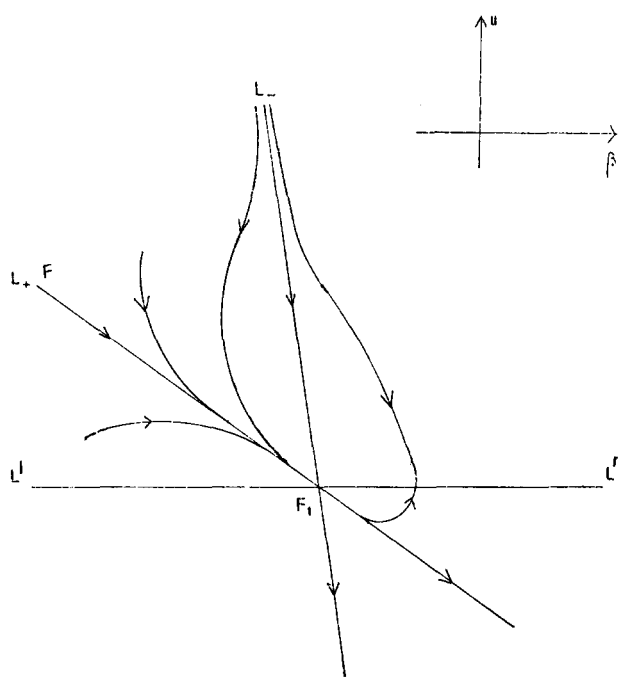

FIG. 2. Qualitative behavior of the dynamical system (12′)–(14′) near the singular point F_1.

The line G intersects the plane L of nonextensibility of solutions $u = -\sqrt{k_2}$ in some point G_0 in the region L^r, which is at a finite distance from the segment I_Z.

Because G_0 depends continuously on parameter k_2 and tends to Z_1 when k_2 tends to k_1, it follows that for $k_2 \approx k_1$ there exists some segment G_X on the line G (beginning from the point G_0) which does not intersect the separatrix Z (see Ref. 12). From this fact and from the presence of the Lyapunov function, it follows that all trajectories of the dynamical system (12′)–(14′) starting from the line G_X, with decreasing parameter z, arrive to the singular line N. This proves the following.

Corollary: All self-similar solutions, which may be matched with the Friedmann solution across a shock wave at $k_2 \approx k_1$ and small enough Mach number, belong to the class of solutions which come from the region $u > 0$ (see Sec. III).

This corollary gives an analytical proof of the numerical results obtained in Ref. 10.

V. SELF-SIMILAR SOLUTIONS WITH TWO EXPANDING SHOCK WAVES

The existence of self-similar solutions with two shock waves in general relativity is connected with the presence of segment I_1 of saddle singular points of the line I. For these points there exists a two-dimensional separatrix L_1 filled with the trajectories T passing through the segment I_1 from supersonic to subsonic domain (see Fig. 3).

We consider two points K_1, K_2 on such trajectory T, at the point K_1 we have $u < -\sqrt{k}$, at the point k_2, $u > -\sqrt{k}$. The points JK_1 and JK_2 correspond to the points K_1, K_2 by means of jump conditions (25). We denote T_1 and T_2, the trajectories passing through the points JK_1 and JK_2 for decreasing and increasing self-similar parameter r, respectively.[2]

The whole self-similar solution is described by three trajectories T_1, T, T_2, and has two shock waves, corresponding to the jumps at the points $JK_1 \to K_1$ and $K_2 \to JK_2$. In general

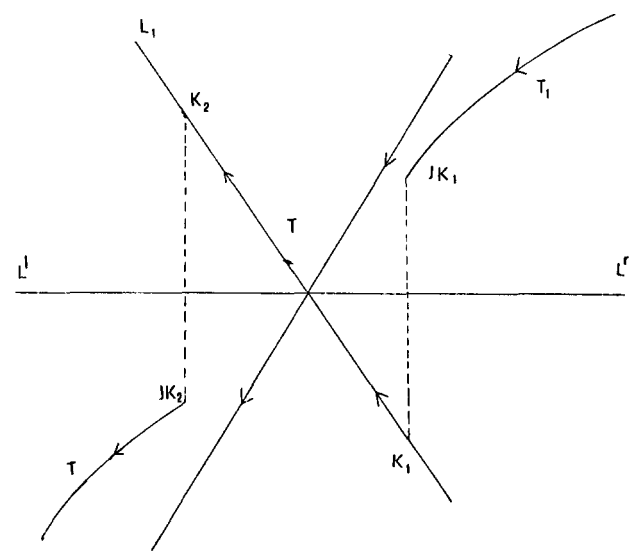

FIG. 3. Solutions with two expanding shock waves.

the trajectory T_1, for decreasing values of parameter r, tends to some point on the segment N and hence its behavior is described like in the Sec. III. But if the point JK_1 belongs to the separatrix Z then the trajectory T_1 tends to the point Z_1 for $r \to 0$ and the corresponding self-similar solution is continued to the center of symmetry without singularity. The trajectory T_2 for increasing values of the parameter r tends to some point on segment DE (see Fig. 1), then it may be continued without singularity in the domain $u > -1$. This trajectory describes the solutions in front of the first expanding shock wave.

These solutions depend on six parameters: one parameter determines the position of the singular point on the segment I_1, two parameters determine the positions of the points K_1, K_2 on the trajectory T, and three parameters k_1, k_2, k_3 determine the state equation $p = k\epsilon$ for three trajectories T_1, T, T_2. By means of variations of these six parameters one may try to obtain a self-similar solution with some extra properties. Some of these extra properties may be that the point JK_2 belongs to the Friedmann trajectory or to the Oppenheimer–Volkov trajectory, and the point JK_1 belongs to the separatrix Z.

The problem of the existence of the points JK_1 and JK_2 with these properties may be solved by means of numerical calculations or by analytic methods at small Mach numbers $M \approx 1$. These new solutions with two expanding shock waves are analogs of the known Landau solution with two shock waves in classical gas dynamics.[13]

VI. SOME QUALITATIVE REMARKS IN THE POLYTROPIC CASE

In this section some qualitative results related to the general dynamical system (12)–(15), which are helpful for the investigation of the solutions described in the next section, will be found. Because of Eqs. (16) and (23) the dynamical system is defined in the region $-1 < u < 1$, $Q > 0$, $L > 0$, $0 < a < \sqrt{\gamma - 1}$, which may be divided in two regions A: $-1 < u < 0$ and B: $0 < u < 1$.

In region A we have the following results.

(i) Equation (16) can be written in the following form:

$$-w + Q^2 - (wQ/u)(u^2 + (a^2/\gamma)(1 - u^2)) < 1 \qquad (16'')$$

and Eq. (18) will give the following bounds for the region A:

$$0 < Q < 1, \quad -1 < w < 0, \quad 0 < u < 1, \quad 0 < a < \sqrt{\gamma - 1}.$$

(ii) The dynamical system changes direction on the hyperplane $u = a$, in fact it is easily seen that the numerator of the right-hand side of Eq. (14),

$$-(1 - u^2)(Q(u^2 - a^2 + 2a^2(1 - u^2 - \gamma)/\gamma) + (w/2)u(1 - a^2) - 2ua^2), \qquad (35)$$

is positive in the region $u < a$ ($\dot{u} < 0$) and in a neighborhood of the hyperplane $u = a$ in the region $u > a$ ($\dot{u} > 0$). Therefore there are no solutions that cross the hyperplane $u = a$ but all solutions exit in both sides of this hyperplane (Fig. 4).

(iii) It is easy to see that in the region $u < a$ there are no singular points and in the region $u > a$ there are only saddle singular points with separatrices belonging to the boundary of phase space. This means that there are no interior solutions starting from some singular point, hence all interior solutions start with a positive value of parameter r from the hyperplane $u = a$.

From (ii) and (iii), as in the barotropic case, the following holds.

Proposition: All trajectories lying in the interior of region $u > 0$ cannot be continued until the center even if a discontinuity (shock wave) is introduced.

Solutions starting from the hyperplane $u = a$ in the side $u < a$ arrive to the region $u < 0$ across the hyperplane $u = 0$ with a finite value r_0 of parameter r, because in this hyperplane there are no singular points of the dynamical system. For these solutions it must be $w(r_0) = a(r_0) = 0$. The first equation follows immediately from Eq. (18), the second one follows from the first and from Eq. (23) by taking into account that by Eq. (16) the function wQ/u cannot tend to $-\infty$ when r tends to r_0.

Following this section we will study the behavior of the dynamical system in the neighborhood of the line N ($w = u = a = 0$). Before making this study it is necessary to regularize the dynamical system on N by taking the new parameter z_1 such that $dz/dz_1 = u(u^2 - a^2)$.

In this way the points of N become singular points for the new dynamical system, but unfortunately they are degenerate (all eigenvalues are zero). This difficulty may be avoided by considering the following new coordinates $x = (Q - \alpha)/a$, $y = w/a$, $z = u/a$, a in a neighborhood of the singular point $Q = \alpha$, $w = u = a = 0$. In these new coordinates the dynamical system becomes

$$\dot{x} = (z^2 - 1)(xa + \alpha)(z(1 - ya - (xa + \alpha)^2) - (y/2)(xa + \alpha)(1 + z^2a^2)) - xF_a/a, \qquad (12'')$$

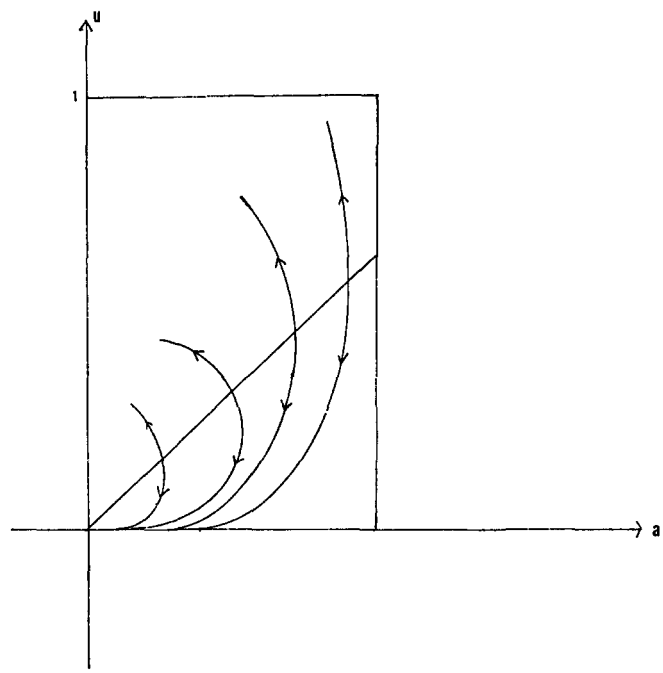

FIG. 4. Behavior of the dynamical system (12)–(15) near the hyperplane $u = a$.

$$\dot{y} = -y((z^2-1)(za(1+ya+(xa+\alpha)^2) + (xa+\alpha)((1+(ya/2))(1+z^2a^2) + (2a^2/\gamma)(1-z^2a^2)) + F_a/a), \quad (13'')$$

$$\dot{z} = -z((1-z^2a^2)((xa+\alpha)(z^2-3+(2/\gamma)(1-z^2a^2)) + (yz/2)(1-a^2) - 2za) + F_a/a), \quad (14'')$$

$$\dot{a} = F_a(x,y,z,a), \quad (15'')$$

where

$$F_a = a(\gamma - 1 - a^2)((yz/4)(1-z^2a^2) - z^3a - (xa+\alpha)(z^2 - (1/\gamma)(1-z^2a^2))).$$

The system (12")–(15") after linearization has the following eigenvalues:

$$\lambda_x = -\alpha(\gamma-1)/\gamma, \quad \lambda_y = \alpha/\gamma, \quad \lambda_z = \alpha(2\gamma-1)/\gamma, \quad \lambda_a = \alpha(\gamma-1)/\gamma. \quad (36)$$

This means that for any α and therefore for any point P of the line N there exists a three-dimensional unstable separatrix that is an invariant three-dimensional manifold filled by trajectories exiting from P. Furthermore for $r \to r_0$, u, $a^{(3\gamma-2)/(\gamma-1)}$, $w^{(3\gamma-2)/\gamma}$ are infinitesimal of the same order. From this and from Eqs. (9), (10), and (17) it follows that for such trajectories, for $r \to r_0$, the pressure tends to a positive constant and the density of energy tends to infinity. By defining the total mass enclosed within the sphere of radius $e^{\tau}r$ as

$$m(\tau,r) = e^{\tau}r(1 + r^2e^{-\nu} - e^{-\lambda})/2, \quad (37)$$

it follows that the function

$$M(r) = 2m/(e^{\tau}r) = (w + (Qw/u)(u^2 + (a^2/\gamma)(1-u^2)))/L \quad (38)$$

must be negative on r_0 because the ratio wa^2/u tends to a negative constant. In Ref. 10 it has been proved that the condition $M(r_0) < 0$ implies the existence of a trapped hypersurface in the interior solution $(0 < r < r_0)$ holding the center of symmetry.[14]

Thus for trajectories coming from the region $u > 0$ we obtain the following conclusions.

(1) As in the barotropic case the only possibility of obtaining a complete solution is to join these solutions at $r = r_0$ with non-self-similar solutions containing the center of symmetry, across a shock wave [contact discontinuity because $u(r_0) = 0$] or to change the topology of interior solution; in the first case the interior solution possesses a trapped surface.

(2) The behavior of these solutions near the contact discontinuity at $r = r_0$ is different from the corresponding barotropic solutions,[11] because in this case the density of energy tends to infinity.

VII. EXPANDING SELF-SIMILAR SHOCK WAVE IN THE FLAT FRIEDMANN UNIVERSE (POLYTROPIC CASE)

In Sec. IV we have considered solutions of the dynamical system (12')–(14'), which are matched with flat Friedmann solution across a shock wave with a small Mach number. In this section we will look for solutions of the general dynamical system (12)–(15) which may be joined to the flat Friedmann solution with dust ($p = 0$) across a shock wave, without restriction on Mach number.

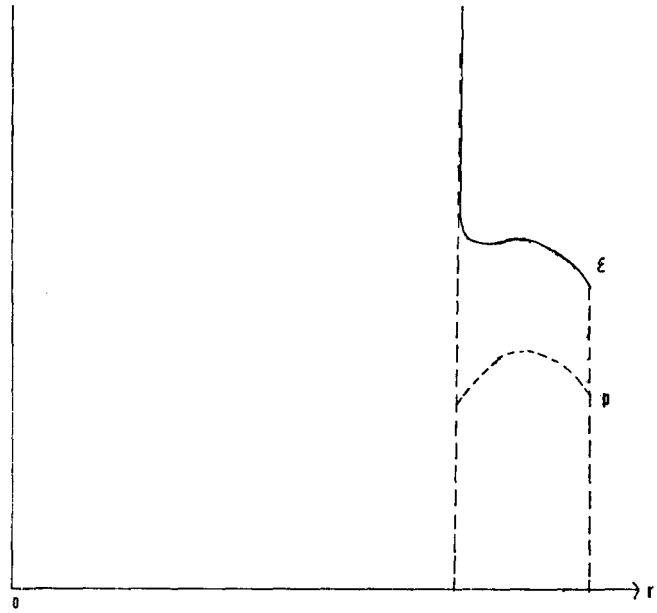

FIG. 5. Behavior of energy density and pressure for the solution of the dynamical system (12)–(15) with $\gamma = \frac{4}{3}$, matched to the Friedmann solution with dust for $u = -0.3$.

In the polytropic case the continuity of Q, w, and L give the following jump conditions:

$$[Q] = [w] = [u + a^2(1-u^2)/(\gamma u)] = 0. \quad (39)$$

As in the barotropic case the first of Eqs. (24) does not give further constraint, but the second becomes

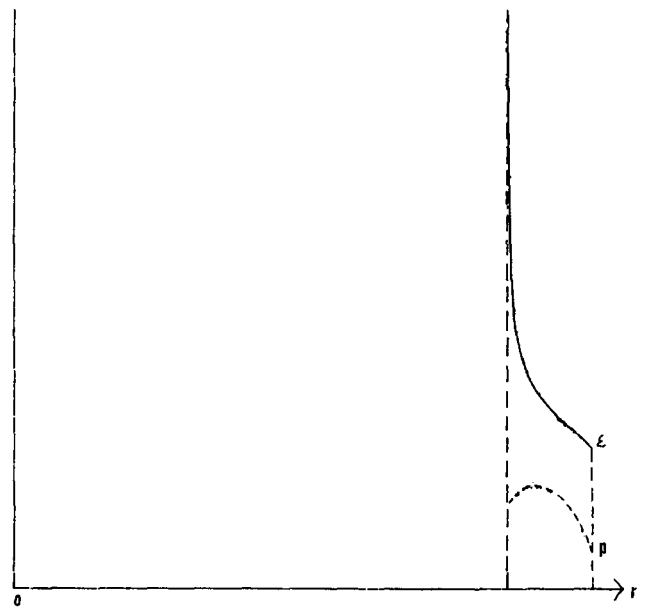

FIG. 6. Like Fig. 5 with $u = -0.2$.

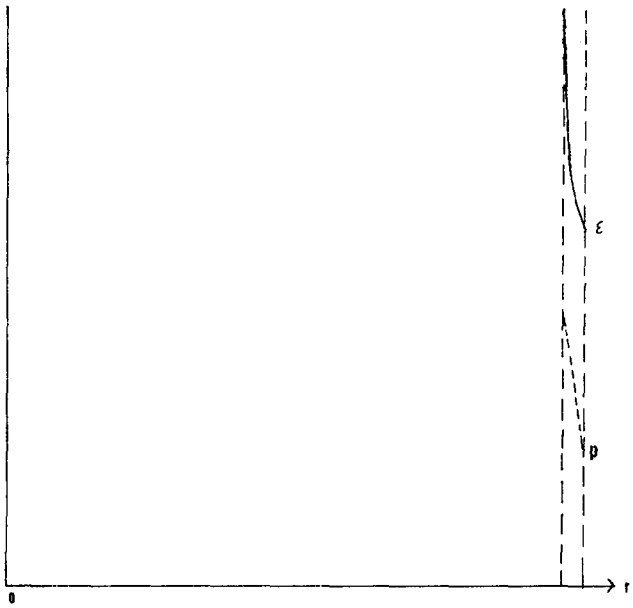

FIG. 7. Like Fig. 5 with $u = -0.05$.

$$(\gamma - 1 - a^2)\sqrt{(1-u^2)}/(\gamma - 1) = 0. \quad (40)$$

Equations (39) and (40) are the jump conditions on a shock wave. The Friedmann solution with dust, is obtained from Eqs. (30) by letting $k = 0$:

$$Q_F = \frac{9r\sigma}{9\sigma^2 + 2r^2}, \quad w_F = \frac{4r^2}{9\sigma^2 + 2r^2}, \quad u_F = -\frac{r}{3\sigma}, \quad (41)$$

where $\sigma(r)$ is defined implicitly by the equation

$$\sigma^2 = c_3(9\sigma^2 - r^2)^{3/2} \quad (42)$$

and c_3 is an integration constant.

By calculating the density of matter (= density of energy) and by taking into account that $a = 0$ it follows that the matching conditions (39) and (40) become

$$Q(r_0) = Q_F(r_0), \quad w(r_0) = w_F(r_0), \quad (43)$$

$$u + a^2(1-u^2)/(\gamma u) = u_F, \quad (44)$$

$$(\gamma - 1 - a^2)\sqrt{1-u^2}/(\gamma - 1) = \sqrt{1-u_F^2}, \quad (45)$$

where it is understood that the variable in Eqs. (44) and (45) are calculated at $r = r_0$ (equation of shock wave).

By using the third equation of (41) and Eq. (42), Eqs. (44) and (45) give

$$a^2 = 2\gamma(\gamma - 1)u^2/((\gamma - 1)^2 + (2\gamma - 1)u^2), \quad (46)$$

$$r_0 = -u(\gamma^2 - 1 - u^2)((\gamma - 1)^2 + (2\gamma - 1)u^2)^2/(9(1-u^2)^{3/2}((\gamma - 1)^2 - u^2)^3) \quad (47)$$

and

$$u_F = u(\gamma^2 - 1 + u^2)/((\gamma - 1)^2 + (2\gamma - 1)u^2). \quad (48)$$

Equations (43), (46), and (47) give the initial data for the interior solution for any choice of u.

From Eq. (46) it follows that $0 < a^2 < \gamma - 1$ if and only if u belongs to the interval $(1-\gamma, 0)$. And from Eq. (48) it follows that $-u_F$ (= velocity of the shock wave with respect to the exterior fluid) is nonzero and less than the velocity of light (= 1) if u is different from 0 and $1 - \gamma$.

Therefore solutions in the interior of the shock wave are parametrized by the variable u belonging to the interior of the interval $(1 - \gamma, 0)$. For some value of u in the previous interval and for $\gamma = \frac{4}{3}$, the corresponding numerical solutions of the system (12)–(15) have been found. These solutions come from the region $u > 0$, then qualitative analysis made in the previous section may be used.

The numerical behavior of the pressure and energy density for any solution is pictured in Figs. 5–7.

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General exact solutions of Einstein equations for static perfect fluids with spherical symmetry

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The gravitational field equations for a spherical symmetric perfect fluid are completely solved. The general analytical solution obtained depends on an arbitrary function of the radial coordinate. As illustrations of the proposed procedure the exterior and interior Schwarzschild solutions are regained.

I. INTRODUCTION

In this paper we derive the whole set of exact spherically symmetric solutions of Einstein gravitational field equations (with cosmological constant) when a perfect fluid is assumed to be the source of the gravitational field.

An extension of the solution to plane and hyperbolic symmetries can easily be obtained and our previous result[1] for the (exact solution of the) plane symmetric case is regained.

In what follows we pose the mathematical problem and then we mimic the procedure used in our recent work[1] to reduce the problem to mere quadratures.

The line element considered here is

$$ds^2 = g^2(x)dt^2 - dx^2 - r^2(x)[d\theta^2 + \sin^2\theta\, d\varphi^2], \tag{1}$$

which represents the most general static line element admitting spherical transformations.

Einstein field equations with cosmological constant are

$$G_{\mu\nu} + \Lambda g_{\mu\nu} = T_{\mu\nu} \tag{2}$$

with

$$G_{\mu\nu} = R_{\mu\nu} - \tfrac{1}{2}g_{\nu\mu}R. \tag{3}$$

In Ref. 1 we proved that if the right-hand side of Eq. (2) models a perfect fluid with pressure p and energy density ρ,

$$T_{\mu\nu} = (\rho + p)u_\mu u_\nu - pg_{\mu\nu}, \tag{4}$$

and whose flow lines are tangent to the unit vector $u^\mu = (1/g)\delta^\mu_0$, the change of variable

$$\tilde{p} = p - \Lambda, \quad \tilde{\rho} = \rho + \Lambda, \tag{5}$$

transforms Eq. (2) into an equivalent system with $\Lambda = 0$. Therefore, twirls can now be dropped keeping in mind that the $\Lambda \neq 0$ case is already included. The field equations (2) for the metric given by (1) are (see, for instance, Ref. 1)

$$\begin{aligned} &2r''/r + r'^2/r^2 - 1/r^2 = -\rho, \\ &r'^2/r^2 + 2r'g'/rg - 1/r^2 = p, \\ &r''/r + g''/g + r'g'/rg = p, \end{aligned} \tag{6}$$

and the equation of hydrostatic support (Bianchi identities) is

$$(\rho + p)(g'/g) + p' = 0, \tag{7}$$

where the prime denotes x differentiation.

II. INTEGRATION

The system of equations can be reaccommodated if the first equation of (6) is multiplied by r^2r' and integrated over x. Then

$$r'^2 = 1 - 2m(r)/r, \tag{8}$$

where

$$\frac{dm}{dr} = \frac{1}{2}\rho r^2. \tag{9}$$

Replacing Eqs. (7) and (8) in the second equation of (6) one obtains

$$(r - 2m)\left(\frac{1}{r^3} - \frac{2}{r^2}\frac{dp}{dr}\frac{1}{\rho + p}\right) = p + \frac{1}{r^2}. \tag{10}$$

Defining

$$G \equiv -(r - 2m)/(p + 1/r^2) \tag{11}$$

Eq. (10) becomes

$$\begin{aligned} &r^3G(G - r^3)\frac{dp}{dr} + r^3(G + r^3)\left(\frac{dG}{dr} + r^2\right)p \\ &\quad + (G + r^3)\left(r^3 + r\frac{dG}{dr} - 2G\right) = 0. \end{aligned} \tag{12}$$

Equation (12) can be integrated at once for $p(r)$ if $G(r)$ is a given function, in fact,

$$\begin{aligned} p(r) = \exp&\left[\int \frac{(G + r^3)(dG/dr + r^2)}{G(r^3 - G)}\right] \\ &\times\left\{p_0 - \int \frac{(G + r^3)(r^3 + r(dG/dr) - 2G)}{r^3G(G - r^3)}\right. \\ &\left.\times\exp\left[-\int \frac{(G + r^3)(dG/dr + r^2)}{G(r^3 - G)}\,dr\right]dr\right\}, \end{aligned} \tag{13}$$

where p_0 is an integration constant.

The function $\rho(r)$ can be obtained with the help of Eq. (9) and the definition of G

$$\rho = \frac{1}{r^2}\left(G\frac{dp}{dr} + \frac{dG}{dr}p - \frac{2G}{r^3} + \frac{dG/dr}{r^2} + 1\right), \tag{14}$$

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where $p(r)$ is given by Eq. (13). The metric coefficient g can be found by direct integration of Eq. (7) and then using Eq. (10) and the definition (11)

$$g^2(r) = g_0^2 \exp\left(-2\int \frac{dp/dr}{\rho + p}\, dr\right)$$

$$= \frac{g_0^2}{r} \exp\left(-\int \frac{r^2}{G}\, dr\right). \tag{15}$$

To complete the integration we can recover the link between the metric coefficient r and the original variable x. From Eq. (8)

$$x = \int \frac{dr}{\sqrt{1 - 2m/r}} \tag{16}$$

with $m(r)$ constructed from Eq. (11).

As we have remarked in our previous work the crucial step to get the general solutions (13)–(16) is the definition (11) of the arbitrary function $G(r)$. It is worthwhile to emphasize that any choice of $G(r)$ does provide a solution to field equations (6), (7) and no spurious solutions are introduced anywhere as it can be straightforwardly shown by replacing p, ρ, g, and r given, respectively, by expressions (13), (14), (15), and (16) in the original field equations. It is rather simple and illustrative to see how the prescription works.

By using the plane symmetric version of the above-depicted procedure,[1] the most general function G that produces a γ law equation of state was found.[2] Also, the associated fluid pressure, energy density, and metric coefficients were explicitly written down. In particular, after a change of variables, the solutions given by Tabensky and Taub,[3] and by Teixeira, Wolk, and Som[4] were reencountered.

III. EXAMPLES

A. Exterior Schwarzschild solution

In the present case, choose for instance

$$G(r) = -r^2(r - 2M) \tag{17}$$

(where M is a constant) and

$$p_0 = 0. \tag{18}$$

Under such conditions

$$r^3 + r\frac{dG}{dr} - 2G = 0 \tag{19}$$

and consequently [see Eq. (13)]

$$p(r) = 0. \tag{20}$$

Equations (14), (19), and (20) imply

$$\rho(r) = 0. \tag{21}$$

Also, comparing Eq. (11) with Eq. (17)

$$m(r) = M. \tag{22}$$

Thus, Eq. (16) can be written as

$$dx^2 = \frac{dr^2}{1 - 2M/r}. \tag{23}$$

Finally, from Eq. (15)

$$g^2 = (1 - 2M/r). \tag{24}$$

As it can be readily recognized, Eqs. (20), (21), (23), and (24) represent the well known exterior Schwarzschild solution.

It is perhaps worthwhile to notice that in this case $\rho + p = 0$ and Eq. (10) seems to loose its meaning. However, by virtue of Eq. (7) the finiteness of the quotient $p'/(p + \rho)$ is ensured if we assume g'/g to be finite everywhere (except for some r).

B. Interior Schwarzschild solution

Now take[5]

$$G = -r^3 \frac{A\sqrt{1 - r^2/R^2} - B(1 - r^2/R^2)}{A\sqrt{1 - r^2/R^2} - B(1 - 3r^2/R^2)}, \tag{25}$$

where A, B, and R are constants.

By choosing $p_0 = 0$ in the expression (13) for $p(r)$, it is found after a lengthy calculation that

$$p(r) = \frac{1}{R^2} \frac{3B\sqrt{1 - r^2/R^2} - A}{A - B\sqrt{1 - r^2/R^2}}. \tag{26}$$

Also, from Eq. (14)

$$\rho(r) = 3/R^2. \tag{27}$$

Finally Eqs. (15) and (16) give

$$g^2(r) = g_0^2 (A - B\sqrt{1 - r^2/R^2})^2, \tag{28}$$

$$h^2(r) \equiv \frac{1}{1 - 2m/r} = \frac{1}{1 - r^2/R^2}. \tag{29}$$

Equations (26)–(29) represent the interior Schwarzschild solution.[6]

As a final comment, let us say that any other solution can be cast in the above scheme as well. In fact, given any metric that solves Eqs. (6) and (7), the associated function G can be obtained from Eq. (15) as

$$G = -r^3 \frac{g^2}{(d/dr)(rg^2)}. \tag{30}$$

The other relevant functions (p,ρ,h^2) are related to G through the above stated formulas.

In Ref. 5 the generating functions G leading to Tolman, Einstein, Schwarzschild–de Sitter, many other known[8] and some new explicit solutions are exhibited.

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Colliding gravitational plane waves with noncollinear polarization. II

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A simple criterion for colliding gravitational plane waves is developed. This colliding wave condition is preserved by a new realization of the Geroch group augmented by a Kramer–Neugebauer involution. A three-parameter generalization of a two-parameter family of solutions with noncollinear polarization discovered recently by Ferrari, Ibañez, and Bruni is presented, and two additional solutions are derived that demonstrate that much larger families are likely to be constructed in the near future.

I. INTRODUCTION

In an earlier paper[1] we discussed the derivation of new colliding wave solutions of the vacuum Einstein solutions from old ones through the use of coordinate and Ehlers transformations. As an example, we gave explicit results for the metric and the curvature tensor of the first new solution obtained by applying such transformations to the famous Nutku–Halil solution.[2] In the collinear limit the new solution reduced to the $n = 2$ solution of the Ferrari–Ibañez family[3] of solutions. (The Kasner parameter n was defined in paper I.) In principle, additional coordinate and Ehlers transformations would yield noncollinear generalizations of all the even n Ferrari–Ibañez solutions. Similarly, starting with the Chandrasekhar–Xanthopoulos $n = 1$ solution,[4] a series of such transformations would in principle yield noncollinear generalizations of all the odd n Ferrari–Ibañez solutions.

As we were going to press we learned that Ferrari, Ibañez, and Bruni[5] had actually obtained closed form expressions for a two-parameter family of colliding wave solutions with noncollinear polarization. Interestingly, for even n their solutions agreed with ours, while for odd n their solutions were distinct. In particular, their $n = 1$ solution was *not* the Chandrasekhar–Xanthopoulos (Kerr) solution. We soon discovered that the Ferrari–Ibañez–Bruni family could easily be extended to a three-parameter family such that all the known solutions were special members of this family. That resolved the mystery, for it became apparent that the Ferrari–Ibañez–Bruni $n = 1$ solution bears the same relation to the Schwarzschild-NUT solution as the Chandrasekhar–Xanthopoulos $n = 1$ solution bears to the Kerr solution. In our three-parameter family the $n = 1$ solution corresponds to Kerr–NUT!

In Sec. II, Eq. (2.30) of this paper we shall describe a simple criterion for distinguishing a colliding wave solution from other solutions. That section will culminate in explicit metrical expressions, Eqs. (2.45)–(2.48), for our three-parameter generalization of the Ferrari–Ibañez–Bruni family of solutions.

It is quite apparent that our three-parameter family of solutions can be further enlarged. In Sec. II we shall describe a simpler realization $G_0(\Sigma_1)$ of a Geroch group[6] of transformations which transform one colliding wave solution into another. That section will culminate in the description of a new three-parameter $n = 2$ solution, Eqs. (3.29)–(3.31), obtained from the Nutku–Halil $n = 0$ solution by employing transformations which are members of our realization of the Geroch group. The new parameter in this solution is denoted by Δ.

In principle, one should be able to extend the three-parameter family of solutions described in Sec. II to a four-parameter family with the additional parameter Δ. For integral values of n one can proceed as follows. One can employ a Kramer–Neugebauer involution[7] to obtain from the three-parameter $n = 2$ solution a new three-parameter $n = 3$ solution. The augmentation of our realization of the Geroch group by the Kramer–Neugebauer involution is formulated in Sec. IV, which culminates in the new three-parameter $n = 3$ solution, Eqs. (4.12) and (4.13). Additional coordinate and Ehlers transformations can, of course, be used to derive analogous three-parameter solutions for arbitrary integer values of n.

It remains to find an effective way to construct the four-parameter generalization (including Δ) of our own three-parameter generalization of the Ferrari–Ibañez–Bruni solutions. In a subsequent paper we shall formulate a homogeneous Hilbert problem, the solution of which may bring this objective within our grasp.

II. A COLLIDING WAVE CONDITION

A. The set CW_1 of vacuum metrics

We shall be considering certain vacuum solutions of the Einstein field equations for which there exist coordinates x^1, x^2, u, v such that the line element has the form

$$g_{ab}(u,v)dx^a dx^b + 2g_{uv}(u,v)du\,dv \quad (a,b = 1,2)\,, \tag{2.1}$$

$\partial/\partial x^1$ and $\partial/\partial x^2$ are Killing vectors, g_{ab} has signature $+\ +$, $g_{uv} < 0$, and

$$\rho := [g_{11}g_{22} - (g_{12})^2]^{1/2} > 0 \tag{2.2}$$

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over the domain of the chart which consists of all (x^1,x^2,u,v) such that $(x^1,x^2)\in\mathbb{R}^2$ and (u,v) is a member of a union of four contiguous regions

$$\mathrm{I}\cup\mathrm{II}\cup\mathrm{III}\cup\mathrm{IV},$$

where

$$\begin{aligned}
\mathrm{I} &:= \{(u,v)\in\mathbb{R}^2:\ u\leqslant 0,\ v\leqslant 0\},\\
\mathrm{II} &:= \{(u,v)\in\mathbb{R}^2:\ u\leqslant 0,\ 0\leqslant v<1\},\\
\mathrm{III} &:= \{(u,v)\in\mathbb{R}^2:\ 0\leqslant u<1,\ v<0\},\\
\mathrm{IV} &:= \{(u,v)\in\mathbb{R}^2:\ 0<\rho(u,v)\leqslant 1,\ 0\leqslant u,\ 0\leqslant v\}.
\end{aligned} \tag{2.3}$$

The intersection of these four regions of $\mathbb{R}^2$ is the singlet set whose element is the origin $(u,v)=(0,0)$. The coordinates x^a have been scaled so that $\rho(0,0)=1$.

One requires, of course, that the metric be continuous over the entire domain. In region I, it is assumed that g_{ab} and g_{uv} are uniform fields; i.e.,

$$\begin{aligned}
&g_{ab}(u,v)=g_{ab}(0,0),\quad g_{uv}(u,v)=g_{uv}(0,0),\\
&\rho(u,v)=\rho(0,0)=1\quad\text{for all } (u,v)\in\mathrm{I}.
\end{aligned}$$

In other words, the space-time domain in which $(u,v)\in\mathrm{I}$ is a closed subregion of Minkowski space whose boundary consists of two null hypersurfaces that intersect at the Euclidean two-surface $u=v=0$. One can always subject the ignorable coordinates x^a to an $\mathrm{SL}(2,R)$ transformation and the null coordinates u,v to a scaling transformation to make

$$g_{ab}(u,v)=\delta_{ab},\quad g_{uv}(u,v)=-1\quad\text{for all } (u,v)\in\mathrm{I}. \tag{2.4}$$

This option will be kept open but not imposed now.

It is next assumed that the metric components in region II depend only on v, while the metric components in region III depend only on u. Thus

$$\begin{aligned}
&g_{ab}(u,v)=g_{ab}(0,v),\\
&g_{uv}(u,v)=g_{uv}(0,v)\quad\text{for all } (u,v)\in\mathrm{II},
\end{aligned} \tag{2.5}$$

and

$$\begin{aligned}
&g_{ab}(u,v)=g_{ab}(u,0),\\
&g_{uv}(u,v)=g_{uv}(u,0)\quad\text{for all } (u,v)\in\mathrm{III}.
\end{aligned} \tag{2.6}$$

Thus regions II and III are each occupied by a p-p type N gravitational field, i.e., a plane-fronted gravitational wave. Consider the timelike coordinate $t=\frac{1}{2}(u+v)$ and spacelike coordinate $s=\frac{1}{2}(u-v)$. One defines "the future" as being in the direction of increasing t. For fixed $t<0$, the two wave fronts are at $s=t$ and at $s=-t$, respectively. As t increases and approaches 0, the spatial "interval" $|2t|$ between the wave fronts decreases until they collide at $t=0$.

We now introduce an assumption which holds only for a restricted set of p-p type N waves in II and III. So far, we have made no particular choice of the null coordinates u and v. We now assume that if we define u and v by the equations

$$\begin{aligned}
&\rho(0,v)=1-v^2\quad\text{in II},\\
&\rho(u,0)=1-u^2\quad\text{in III},
\end{aligned} \tag{2.7}$$

then the metric components in these regions are C^2-differentiable[8] functions over the intervals $0\leqslant v<1$ and $0\leqslant u<1$, respectively. We shall adhere to the choices (2.7) in this paper.

We now come to the region occupied by the scattered waves; viz., IV. The field equation which governs ρ is

$$\rho_{uv}:=\frac{\partial^2\rho}{\partial u\,\partial v}=0.$$

Hence, from Eqs. (2.7),

$$\rho=1-u^2-v^2\quad\text{in IV}. \tag{2.8}$$

We next seek a C^2-differentiable solution in IV of the vacuum field equations for $g_{ab}(u,v)$ and $g_{uv}(u,v)$. This must satisfy the continuity conditions for the metric at the bounding null hypersurface at $u=0$ and $v=0$, respectively; i.e., the solution must match the prescribed $g_{ab}(0,v)$, $g_{uv}(0,v)$ over the interval $0\leqslant v<1$ and the prescribed $g_{ab}(u,0)$, $g_{uv}(u,0)$ over $0\leqslant u<1$. Moreover, the solution must satisfy the requirement $g_{uv}(u,v)<0$ at all (u,v) in IV. Such solutions do not exist in all cases.

Definition: CW_1 will denote the set of all vacuum metrics that satisfy all of the conditions prescribed above in Sec. II.

Our main interest in this paper will be the members of CW_1 for which colliding wave polarizations are not collinear. So far, every explicitly known vacuum metric regarded as representing the collision of two plane-fronted gravitational waves with noncollinear polarizations is a member of CW_1.

B. The field equations

The field equations governing the metrical components g_{ab} can be reduced to the Ernst equation

$$F(d*\rho\,dE)=\rho\,dE(*\,dE), \tag{2.9}$$

where E is the complex potential

$$\begin{aligned}
&E=F+i\omega:=(g_{22})^{-1}(\rho+ig_{12}),\\
&F:=\mathrm{Re}\,E,
\end{aligned} \tag{2.10}$$

and $*$ is a two-dimensional duality operator such that

$$*du=du,\quad *dv=-dv. \tag{2.11}$$

In terms of u and v, Eq. (2.9) becomes

$$F[E_{uv}-\rho^{-1}(uE_v+vE_u)]=E_uE_v \tag{2.12}$$

over the region IV.

The only remaining independent field equations are those that can be used to compute g_{uv} when E is given:

$$\begin{aligned}
&2u\Gamma_u=1-\rho|E_u/2F|^2,\\
&2v\,\Gamma_v=1-\rho|E_v/2F|^2,
\end{aligned} \tag{2.13}$$

where Γ is the real field defined by

$$-(\rho)^{1/2}g_{uv}=\exp(2\Gamma). \tag{2.14}$$

Equation (2.12) guarantees that the integrability condition for Eqs. (2.13) is satisfied. The solution of Eqs. (2.13) in an instructive form will be given later in Sec. II.

C. The field equations in terms of $\mathscr{E}$

The Ernst potential

$$\mathscr{E}=f+i\chi,\quad f:=\mathrm{Re}\,\mathscr{E}:=-g_{22} \tag{2.15}$$

may be defined in terms of E by the equations

$$fF=-\rho,\quad f^{-1}\,d\chi=-F^{-1}*d\omega. \tag{2.16}$$

The Ernst equation (2.9) guarantees that the integrability condition for the second Eq. (2.16) is satisfied. As is well known, $\mathscr{E}$ is also a solution of the Ernst equation, and Eqs. (2.13) are expressible as

$$2u\,\gamma_u = 1 - \rho|\mathscr{E}_u/2f|^2\,,$$
$$2v\,\gamma_v = 1 - \rho|\mathscr{E}_v/2f|^2\,, \tag{2.17}$$

where γ is defined by

$$-g_{22}g_{uv} = \exp(2\gamma)\,. \tag{2.18}$$

The reasons for introducing the potential $\mathscr{E}$ as well as the potential E are to be found in various methods that have been developed for transforming given solutions of the Ernst equation into new solutions of the equation. In particular, as we shall discuss in detail in Sec. III, new colliding wave solutions with any desired finite number of parameters can be constructed by alternately subjecting E and $\mathscr{E}$ to certain rational linear transformations. This is equivalent to a method originally devised by Geroch.[6]

D. The determination of the colliding wave solution by $E(u,0)$ and $E(0,v)$

As is known from the theory of quasilinear hyperbolic equations such as Eq. (2.12), the solution $E(u,v)$ in the scattered wave region is uniquely determined by its values $E(u,0)$, $E(0,v)$ on the respective null hypersurfaces which constitute the interfaces between the colliding waves and the scattered wave. In particular, the first partial derivatives on the interfaces; viz., $E_v(u,0)$, $E_u(0,v)$ are uniquely determined by $E(u,0)$ and $E(0,v)$, respectively. Specific equations which give these first partial derivatives in terms of $E(u,0)$ and $E(0,v)$ are of some interest and will now be derived.

The derivations proceed by first setting $v=0$ in Eq. (2.12). The result is an ordinary differential equation that can be expressed in the form

$$\frac{d}{du}\left\{\ln\left[\frac{UE_v(u,0)}{F(u,0)}\right]\right\} = \frac{i\omega_u(u,0)}{F(u,o)}\,,$$

where the capital letters U and V will be used to designate the non-negative valued fields

$$U := (1-u^2)^{1/2}, \quad V := (1-v^2)^{1/2}\,. \tag{2.19}$$

By setting $u=0$ in Eq. (2.12) a similar ordinary differential equation is obtained for $E_u(0,v)$. Integration of these ordinary differential equations gives us our final results,

$$\frac{UE_v(u,0)}{F(u,0)} = \frac{E_v(0,0)}{F(0,0)}\left\{\exp\int_0^u da\left[\frac{i\,\omega_a(a,0)}{F(a,0)}\right]\right\},$$
$$\frac{VE_u(0,v)}{F(0,v)} = \frac{E_u(0,0)}{F(0,0)}\left\{\exp\int_0^v db\left[\frac{i\,\omega_b(0,b)}{F(0,b)}\right]\right\}. \tag{2.20}$$

Equations similar to the above hold for $\mathscr{E}$; these are simply obtained by replacing E by $\mathscr{E}$, F by f and ω by χ in Eqs. (2.20). Moreover, from Eq. (2.16) one obtains

$$\frac{\mathscr{E}_u}{f} + \frac{E_u}{F} = -\frac{2u}{\rho}\,, \quad \frac{\mathscr{E}_v}{f} + \frac{E_v^*}{F} = -\frac{2v}{\rho}\,. \tag{2.21}$$

Therefore,

$$\mathscr{E}_u(0,v)/f(0,v) = -E_u(0,v)/F(0,v)\,,$$
$$\mathscr{E}_v(u,0)/f(u,0) = -E_v^*(u,0)/F(u,0)\,. \tag{2.22}$$

From Eqs. (2.20) and (2.22) we obtain the following relations, which will be used later:

$$k := |E_v(0,0)/2F(0,0)|^2 = |UE_v(u,0)/2F(u,0)|^2 = |U\mathscr{E}_v(u,0)/2f(u,0)|^2\,,$$
$$l := |E_u(0,0)/2F(0,0)|^2 = |VE_u(0,v)/2F(0,v)|^2 = |V\mathscr{E}_u(0,v)/2f(0,v)|^2\,. \tag{2.23}$$

The particular case of colliding wave with *collinear* polarization is defined by the statement that there exists a choice of the ignorable coordinates x^a such that g_{12} vanishes at all points. In this case, $\omega=0$ and one can select the arbitrary additive constants in χ so that $\chi=0$ as well. Upon introducing the real scalar field ψ defined by

$$-\mathscr{E} = g_{22} = \exp(2\psi)\,, \tag{2.24}$$

one finds that the Ernst equations for E and for $\mathscr{E}$ are each equivalent to the single linear equation

$$\psi_{uv} - \rho^{-1}(u\psi_v + v\psi_u) = 0\,. \tag{2.25}$$

Moreover, Eqs. (2.23) become

$$k = [\psi_v(0,0)]^2 = [U\psi_v(u,0)]^2\,,$$
$$l = [\psi_u(0,0)]^2 = [V\psi_u(0,v)]^2\,. \tag{2.26}$$

E. A necessary and sufficient condition for a solution of the Ernst equation to yield a member of CW_1

Let E by any solution of the Ernst equation over the domain

$$\{(u,v)\in\mathbb{R}^2:\ 0\leqslant u^2+v^2<1,\ 0\leqslant u,\ 0\leqslant v\}\,,$$

such that E is of differentiable class C^2 and such that $F(u,v) := \mathrm{Re}\,E(u,v) > 0$ for all (u,v) in the domain. From the Ernst equation (2.12), one can readily prove that

$$\frac{\partial}{\partial u}(\rho F^{-2}|E_v|^2) = v\,F^{-2}(E_uE_v^* + E_u^*E_v)\,,$$
$$\frac{\partial}{\partial v}(\rho F^{-2}|E_u|^2) = uF^{-2}(E_uE_v^* + E_u^*E_v)\,. \tag{2.27}$$

Now let us introduce the scalar field

$$\Lambda(u,v) := \frac{1}{4}\int_0^u da\int_0^v db\,[F(a,b)]^{-2}[E_a(a,b)E_b^*(a,b) + E_a^*(a,b)E_b(a,b)]\,. \tag{2.28}$$

Then, from Eqs. (2.23) and (2.27), we obtain

$$\tfrac{1}{4}\rho F^{-2}|E_v|^2 - l = v\Lambda_v\,,$$
$$\tfrac{1}{4}\rho F^{-2}|E_u|^2 - k = u\Lambda_u\,.$$

Substitution of the above into Eqs. (2.13) yields

$$\Gamma_u = (1-k)/u - \Lambda_u, \quad \Gamma_v = (1-l)/v - \Lambda_v\,.$$

Hence, from Eqs. (2.14), one obtains the following result for g_{uv}:

$$f_{uv} = -(\mathrm{const})(\rho)^{-1/2}u^{1-k}v^{1-l}e^{-2\Lambda}\,. \tag{2.29}$$

The positive constant factor in g_{uv} is arbitrary unless one imposes an auxiliary condition to fix it.

It is apparent from Eq. (2.29) that not every E yields a g_{uv} which fits our definition of the class CW_1 of colliding wave solutions. The following key theorem results.

Theorem: E determines a metric in CW_1 by the relation

$$E = (g_{22})^{-1}(\rho + ig_{12})$$

if and only if

$$k = l = 1 . \tag{2.30}$$

Let us consider examples.

F. Some old examples of Ernst potentials that yield colliding wave solutions in CW_1 and other examples that fail in that respect

An Ernst potential which satisfies the conditions $k = l = 1$ is the Kerr metric $\mathscr{E}$ which is given by

$$-\mathscr{E}^* = (1-\xi)(1+\xi)^{-1}, \tag{2.31}$$

where

$$\begin{aligned} &\xi := px + iqy , \\ &x := uV + vU, \quad y = uV - vU , \end{aligned} \tag{2.32}$$

and where the real parameters q and p are related by

$$p^2 + q^2 = 1 . \tag{2.33}$$

The colliding wave solution corresponding to this Ernst potential wave analyzed in depth by Chandrasekhar and Xanthopoulos.[4]

Another example is the Nutku–Halil solution,[2] for which Chandrasekhar and Ferrari[9] observed that

$$E = (1-\xi)(1+\xi)^{-1}, \tag{2.34}$$

which equals the Kerr $-\mathscr{E}^*$ given by Eq. (2.31).

The potential given by Eqs. (2.34) is one member of a larger family of Ernst equation solutions called the *Tomimatsu–Sato* (TS) *family*[10] and which involves an additional real parameter δ. $\delta = 0$ yields Minkowski space; $\delta = 1$ yields the potential (2.34); and $\delta = -1$ yields (2.34) with ξ replaced by $-\xi$. The fact is that the only members of the TS family for which $k = l = 1$ are those for which $\delta^2 = 1$.

The TS family Ernst potentials are very complicated. Let us, therefore, look at the Zipoy–Voorhees[11,12] (ZV) family, which is the collinear version of the TS family. For the ZV family,

$$\psi = \frac{\delta}{2}\ln\frac{1+x}{1-x} \quad \text{or} \quad \psi = \frac{\delta}{2}\ln\frac{1-y}{1-y} . \tag{2.35}$$

A brief calculation employing Eqs. (2.26) and (2.32) yields

$$k = l = \delta^2 .$$

Thus the only members of the ZV family in CW_1 are the Khan–Penrose[13] (collinear specialization of Nutku–Halil) and Schwarzschild solutions, for which

$$E = \exp(2\psi) \quad \text{and} \quad \mathscr{E} = -\exp(2\psi) ,$$

respectively, where ψ is given by Eqs. (2.35) with $\delta = \pm 1$.

As an example which does not satisfy the colliding wave condition, consider the Kasner solutions, for which

$$\mathscr{E} = -\rho^{1-n} = -g_{22} .$$

It is clear that $k = l = 0$. *In fact, any Ernst potential that is expressible as a function of the Weyl canonical coordinates*

$$z = u^2 - v^2, \quad \rho = 1 - u^2 - v^2 \tag{2.36}$$

and is an analytic function of z *and* ρ *in a neighborhood of* $(z,\rho) = (0,1)$ *satisfies* $k = l = 0$ *and cannot, therefore, yield a member of* CW_1. The reader can easily prove this assertion.

G. Recent examples of members of CW_1: A new three-parameter family of colliding wave solutions

The Nutku–Halil solution is itself a member of a two-parameter family of noncollinear members of CW_1 which has been obtained by Ferrari, Ibañez, and Bruni.[5] In paper I we reported our discovery of a three-parameter extension of their family, the derivation of which will be given in a sequel to the present paper. The Ernst potentials E and $\mathscr{E}$ of our three-parameter family are given by

$$E(n,\nu,\nu') = \rho^n T(n+1,\nu',\nu)/T(n-1,\nu',\nu) , \tag{2.37}$$

$$\mathscr{E}(n,\nu,\nu') = \rho^{1-n}[T(n-2,\nu,\nu')/T(n,\nu,\nu')]^* , \tag{2.38}$$

where n, ν, ν' are any real numbers, where we let

$$\begin{aligned} &p := \cos\nu, \quad q := \sin\nu , \\ &p' = \cos\nu', \quad q' := \sin\nu' , \end{aligned} \tag{2.39}$$

and where

$$\begin{aligned} T(n,\nu,\nu') := \frac{1}{2}X\Big[&(p+p')\Big(\frac{1-x}{1+x}\Big)^{n/2} \\ &+ (p-p')\Big(\frac{1+x}{1-x}\Big)^{n/2}\Big] \\ + \frac{1}{2}Y\Big[&(q+q')\Big(\frac{1-y}{1+y}\Big)^{n/2} \\ &+ (q-q')\Big(\frac{1+y}{1-y}\Big)^{n/2}\Big] , \end{aligned} \tag{2.40}$$

where x and y were defined by Eqs. (2.32), and

$$X := (1-x^2)^{1/2}, \quad Y := (1-y^2)^{1/2} . \tag{2.41}$$

When $q' = 0$ and $p' = 1$, i.e., $\nu' = 0$, the above family reduces to the one found by Ferrari *et al.*, except that we should caution that their parameter p differs from ours.

When $n=0$ in Eqs. (2.37), (2.38), and (2.40), one obtains the Nutku–Halil solution. The parameter ν' is not essential for the Nutku–Halil solution, since it can be removed by an SL(2,R) transformation of the coordinates x^a. However, both ν and ν' are essential parameters for all $n\neq 0$.

When $|n|=1$ in Eqs. (2.37), (2.38), and (2.40), one obtains the Kerr–NUT family, *except that we should warn the reader that it is ν which is the* NUT *parameter in this case.* (Therefore the $n=1$ member of the solutions of Ferrari *et al.* is not the Kerr metric; it is the Schwarzschild–NUT metric.)

Finally, when $n=2$ and $\nu'=0$ in Eqs. (2.37), (2.38), and (2.40), one obtains a solution reported in paper I. When $n=2$, one obtains a specialized version of a three-parameter family which we shall give in Sec. IV.

In evaluating the metric tensor it is convenient to express Eq. (2.37) in the form

$$E=AB^{-1}, \tag{2.42}$$

where

$$\begin{aligned} A&=\rho^{n(n+2)/4}T(n+1,\nu',\nu)\,,\\ B&=\rho^{n(n-2)/4}T(n-1,\nu',\nu)\,, \end{aligned} \tag{2.43}$$

and $T(n,\nu,\nu')$ is defined by Eq. (2.40).

The metric tensor components g_{ab}, g_{uv} are computed from Eqs. (3.7) and (3.9) in paper I. The components g_{ab} in region IV are there expressed in the form

$$g_{11}=\rho K/N,\quad g_{12}=\rho L/N,\quad g_{22}=\rho M/N. \tag{2.44}$$

We obtain

$$\begin{aligned} N&=\mathrm{Re}\,(AB^*)\\ &=\rho^{n^2/2}\frac{1}{4}\left\{X^2\left[(p+p')^2\left(\frac{1-x}{1+x}\right)^n\right.\right.\\ &\quad\left.+(p-p')^2\left(\frac{1+x}{1-x}\right)^n\right]+Y^2\left[(q+q')^2\left(\frac{1-y}{1+y}\right)^n\right.\\ &\quad\left.\left.+(q-q')^2\left(\frac{1+y}{1-y}\right)^n\right]+2(q^2-q'^2)(x^2-y^2)\right\}\\ &=\rho^{n^2/2}|T(n,\nu,\nu')|^2\,, \end{aligned} \tag{2.45}$$

$$K=|A|^2=\rho^{(n^2/2)+n}|T(n+1,\nu',\nu)|^2\,, \tag{2.46}$$

$$M=|B|^2=\rho^{(n^2/2)-n}|T(n-1,\nu',\nu)|^2\,, \tag{2.47}$$

$$\begin{aligned} L&=\mathrm{Im}(AB^*)\\ &=\rho^{n^2/2}\frac{1}{2}\left\{(x-y)\left[(p+p')(q+q')\left(\frac{1-x}{1+x}\right)^{n/2}\right.\right.\\ &\quad\times\left(\frac{1-y}{1+y}\right)^{n/2}-(p-p')(q-q')\left(\frac{1+x}{1-x}\right)^{n/2}\\ &\quad\left.\times\left(\frac{1+y}{1-y}\right)^{n/2}\right]+(x+y)\left[(p-p')(q+q')\right.\\ &\quad\times\left(\frac{1+x}{1-x}\right)^{n/2}\left(\frac{1-y}{1+y}\right)^{n/2}-(p+p')(q-q')\\ &\quad\left.\left.\times\left(\frac{1-x}{1+x}\right)^{n/2}\left(\frac{1+y}{1-y}\right)^{n/2}\right]\right\}. \end{aligned} \tag{2.48}$$

To obtain the explicit expression for $|T(n+1,\nu',\nu)|^2$ in Eq. (2.46), simply replace n by $n+1$ and interchange p with p' and q with q' in that expression for $|T(n,\nu,\nu')|^2$, which is given by Eq. (2.45). A like rule yields $|T(n-1,\nu',\nu)|^2$ in Eq. (2.47).

The remaining metrical component g_{uv} is

$$g_{uv}=-\rho^{-1/2}N/(UV)\,, \tag{2.49}$$

where N is given by Eq. (2.45).

Interesting relations between members of the family corresponding to different n are given in Secs. III and IV.

III. A REALIZATION OF A GEROCH GROUP

A. Objectives

Regarding the set of metrics CW_1, our ultimate goal is to find an effective way of constructing an exact solution for the metric in the scattered wave region IV when the metrics of the two plane-fronted waves in regions II and III are given. Equivalently, we would like to be able to obtain $\mathscr{E}(u,v)$ when $\mathscr{E}(0,v)$ and $\mathscr{E}(u,0)$ are given.

If the polarizations of the p-p waves are collinear, a general solution of this problem is obtained by applying Riemann's method to the hyperbolic linear equation (2.25), and this has already been done under varying assumptions by Szekeres[16] and by Xanthopoulos.[17] When the polarizations are not collinear, the quasilinear Ernst equation cannot be converted by any known way to an equivalent linear partial differential equation involving only a finite number of dependent and independent variables. One must seek a different approach.

The approach which we are seeking is a generalization of methods that several people, including two of the present authors, have applied to stationary axisymmetric gravitational fields in the Einstein theory. There, the problem is to determine the Ernst potential $\mathscr{E}(z,\rho)$ when its values $\mathscr{E}(z,0)$ on the axis are given.

In the particular method developed by Hauser and Ernst,[18] a 2×2 matrix function $u(t)$ of a complex variable t is constructed by algebraic means from $\mathscr{E}(z,0)$. The function $u(t)$ is an element in a realization of a group central to our entire discussion. This group was first effectively formulated and applied by Kinnersley and Chitre[15] and is an extension of one originally conceived by Geroch.[6]

The method continues with the use of $u(t)$ to construct the kernel of a Fredholm equation of the second kind or an equivalent homogeneous Hilbert problem whose solution is a 2×2 matrix function $F(t,z,\rho)$. The Ernst potential $\mathscr{E}(z,\rho)$ is one of the matrix elements of $\partial F/\partial t$ at $t=0$. [Also, the elements of the real part of $\partial F/\partial t$ at $t=0$ are the negatives of the metric components $g_{ab}(z,\rho)$.]

Thus the problem of determining $\mathscr{E}(z,\rho)$ from $\mathscr{E}(z,0)$ is reduced to the (not necessarily easy) problem of solving a linear integral equation or homogeneous Hilbert problem. This method may be described as a synthesis of a group theoretical theme of Geroch and a type of inverse scattering technique. We wish to formulate a similar synthesis for the colliding wave problem.

To approach the ultimate goal we have described above, we must first go through several stages. In this section we shall present the first stage which is *to provide a realization of the original Geroch group, specifically one suitable for our*

present purposes. The Geroch group is infinite dimensional and can be used to construct colliding wave solutions with any desired finite number of parameters. In fact, we shall give a simple example of the way in which the group realization is used to build a new solution out of a given known one. *However, we stress that our central objective here is to provide the first link in a conceptual chain.* We are not concerned in this paper with providing any effective modes of calculation; that will come in sequels.

B. A realization of SL(2,R) that induces rational linear transformations of E

The Geroch group is constructed by taking the free product of two groups of transformations, both of which are realizations of SL(2,R), and both of which transform a vacuum metric with a line elment of the form (2.1) into the same vacuum metric or into another one with a line element of the form (2.1). In this subsection we shall describe one of these realizations of SL(2,R).

We start by considering the group of SL(2,R) transformations of the ignorable coordinates, or, equivalently, the set of transformations

$$\begin{pmatrix} \dfrac{\partial}{\partial x^{1'}} \\ \dfrac{\partial}{\partial x^{2'}} \end{pmatrix} = w \begin{pmatrix} \dfrac{\partial}{\partial x^{1}} \\ \dfrac{\partial}{\partial x^{2}} \end{pmatrix}, \tag{3.1}$$

where w is any member of SL(2,R),

$$w = w^* = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}, \quad \alpha\delta - \beta\gamma = 1 . \tag{3.2}$$

Correspondingly, the metric component g_{uv} remains invariant while the metric components g_{ab} undergo the transformation into

$$h' = whw^T, \quad \text{where } h := \begin{pmatrix} g_{11} & g_{12} \\ g_{21} & g_{22} \end{pmatrix}. \tag{3.3}$$

As a result, E as defined by Eq. (2.10) becomes

$$E' = i(\alpha E + i\beta)(\gamma E + i\delta)^{-1}, \tag{3.4}$$

where

$$E' := (g'_{22})^{-1}(\rho + ig'_{12}) .$$

Thus we obtain, in general, a new solution of the Ernst equation, though, of course, *the transformation has not changed the physical field*; i.e., *the transformation has not altered the value of the line element at any point of the manifold. It is the same space-time.*

What about the way $\mathscr{E}$ transforms under this group? From the defining relations (2.6) between E nd $\mathscr{E}$, one deduces that

$$\begin{aligned} \mathscr{E}'(u,v) = & -[\rho/F'(u,v)] + i\chi'(0,0) \\ & + i\left\{ \int_0^u da \left[\frac{(1-a^2)\omega'_a(a,0)}{F'(a,0)^2} \right] \right. \\ & \left. + \int_0^v db \left[\frac{(1-u^2-b^2)\omega'_b(u,b)}{F'(u,b)^2} \right] \right\}, \end{aligned} \tag{3.5}$$

where $F' = \operatorname{Re} E'$ and $\omega' = \operatorname{Im} E'$ are given by Eq. (3.4) and where $\chi'(0,0)$ is arbitrary. Thus the transformation of $\mathscr{E}$ is *nonlocal.* Incidentally, *we shall henceforth adopt the convention*

$$\chi'(0,0) = \chi(0,0) \tag{3.6}$$

in Eq. (3.5). [However, $\omega'(0,0)$ does not generally equal $\omega(0,0)$ in Eq. (3.4).]

Before we proceed with our discussion of the group, let us pause to introduce two helpful notations.

Definition: Σ will denote the set of all ordered pairs $(E,\mathscr{E})$ of C^2-differentiable solutions of the Ernst equation such that (1) region IV is the domain of E and $\mathscr{E}$; (2) $F(u,v) := \operatorname{Re} E(u,v) > 0$ and $f(u,v) := \operatorname{Re} \mathscr{E}(u,v) < 0$ for all (u,v) in IV; (3) the relations (2.6), where $E = F + i\omega$ and $\mathscr{E} = f + i\chi$, hold throughout IV.

For each $(E,\mathscr{E})$ in Σ, there is exactly one metric (2.1) such that

$$E = (g_{22})^{-1}(\rho + ig_{12}) .$$

Definition: For each w in SL(2,R), let $\gamma_1(w)$ denote that mapping whose domain is Σ such that

$$\gamma_1(w)(E,\mathscr{E}) = (E',\mathscr{E}') , \tag{3.7}$$

where E' is given by Eqs. (3.2) and (3.4) and where $\mathscr{E}'$ is given by Eqs. (3.5) and (3.6).

We shall also find it helpful to use the *mnemonic symbols*

$$\gamma_1(w)E \quad \text{and} \quad \gamma_1(w)\mathscr{E}$$

to stand for the first member E' and the second member $\mathscr{E}'$ in the ordered pair (3.7).

Let us look at two examples of $\gamma_1(w)$. A much used set of generators of SL(2,R) consists of its elements

$$w_\Delta := \begin{pmatrix} 1 & \Delta \\ 0 & 1 \end{pmatrix} \quad \text{for all } \Delta \in \mathbb{R}^1 , \tag{3.8a}$$

$$\epsilon := \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{3.8b}$$

From the definition of $\gamma_1(w)$ given by Eqs. (3.7), (3.4), (3.2), (3.5), and (3.6), one can see that

$$\gamma_1(w_\Delta)(E,\mathscr{E}) = (E + i\Delta, \mathscr{E}) , \tag{3.9a}$$

$$\gamma_1(\epsilon)(E,\mathscr{E}) (E^{-1},\mathscr{E}') . \tag{3.9b}$$

As regards $\mathscr{E}' = \gamma_1(\epsilon)\mathscr{E}$ in Eqs. (3.9b), the expression for it is not trivial and is not required here. Note, by the way, that

$$\gamma_1(\pm I)(E,\mathscr{E}) = (E,\mathscr{E}) ;$$

i.e., $\gamma_1(\pm I)$ is the identity mapping on Σ.

In the following theorem, $\circ$ denotes the mapping composition symbol, and the factors in a composition are read from right to left.

Theorem: (1) $\gamma_1(w)$ maps Σ onto Σ and is one-to-one.
(2) For all w and v in SL(2,R),

$$\gamma_1(w) \circ \gamma_1(v) = \gamma_1(wv) . \tag{3.10}$$

(3) $F^{-2}(dE \otimes dE^*)$ is invariant under $\gamma_1(w)$. (3.11)

We shall not supply any details of the simple proof of the above well-known statements. Equation (3.11) is most easily proved by showing that it is true for $w = w_\Delta$ and ϵ. Note that $|E_u|^2$ and $|E_v|^2$ are components of the tensor product in Eq. (3.11). Therefore, the following corollary is implied by Eqs. (2.23) and (3.11).

Corollary: The colliding wave condition $k=l=1$ is preserved by $\gamma_1(w)$.

$\gamma_1(w)$ is our first realization of SL(2,R). We next consider the second realization of SL(2,R) which will be used to construct a realization of the Geroch group.

C. A realization of SL(2,R) that induces rational linear transformations of $\mathscr{E}$

Let us start by inspecting the simple transformation

$$\mathscr{E}\to\mathscr{E}+i\Delta\,. \tag{3.12}$$

$\mathscr{E}+i\Delta$ is also a solution of the Ernst equation. Note that $E\to E$ under this transformation.

Next consider

$$\mathscr{E}\to\mathscr{E}^{-1}\,. \tag{3.13}$$

The reader can easily verify that $\mathscr{E}'=\mathscr{E}^{-1}$ is also a solution of the Ernst equation such that Re $\mathscr{E}'<0$. *This is the transformation which was applied to the Nutku–Halil $\mathscr{E}$ potential in paper I in order to construct a new solution. It is the first transformation, among those explicitly considered so far in Sec.* III, *which actually changes the space time into a new one.*

Repeated alternate applications of the transformations (3.12) and (3.13), with different values of the parameters Δ, generate the group of rational linear transformations

$$\mathscr{E}\to\mathscr{E}''=i(\alpha\mathscr{E}+i\beta)(\gamma\mathscr{E}+i\delta)^{-1}\,, \tag{3.14}$$

where $\alpha\delta-\beta\gamma=1$. It is apparent at this point that much of what we did in Sec. III B is applicable when E and $\mathscr{E}$ are interchanged. Therefore, we proceed onwards to a formal development that parallels what we did in Sec. III B.

Definition: For each w in SL(2,R), let $\gamma_2(w)$ denote that mapping whose domain is Σ such that

$$\gamma_2(w)(E,\mathscr{E})=(E'',\mathscr{E}'')\,, \tag{3.15}$$

where $\mathscr{E}''$ is given by Eq. (3.14) and where

$$\begin{aligned}E''(u,v)=&-[\rho/f''(u,v)]+i w(0,0)\\&+i\left\{\int_0^u da\left[\frac{(1-a^2)\chi_a''(a,0)}{f''(a,0)^2}\right]\right.\\&\left.+\int_0^v db\left[\frac{(1-u^2-b^2)\chi_b''(u,b)}{f''(u,b)^2}\right]\right\}.\end{aligned} \tag{3.16}$$

$f''=\mathrm{Re}\,\mathscr{E}''$ and $\chi''=\mathrm{Im}\,\mathscr{E}''$ are given by Eq. (3.14). We have fixed the constant of integration in E'' by the requirement that

$$\omega''(0,0)=\omega(0,0)\,.$$

The reader should compare Eqs. (3.14) and (3.16) with Eqs. (3.4)–(3.6) and with Eq. (3.7).

We shall find it helpful to use the *mnemonic symbols* $\gamma_2(w)E$ and $\gamma_2(w)\mathscr{E}$ to stand for the first member E'' and the second member $\mathscr{E}''$ in the ordered pair (3.15).

The transformations (3.12) and (3.13) are now expressible as

$$\gamma_2(w_\Delta)(E,\mathscr{E})=(E,\mathscr{E}+i\Delta)\,, \tag{3.17a}$$

$$\gamma_2(\epsilon)(E,\mathscr{E})=(E'',\mathscr{E}^{-1})\,, \tag{3.17b}$$

which should be compared with Eqs. (3.9). Furthermore, we have the following theorem and corollary corresponding to the ones given in Sec. III B.

Theorem: (1) $\gamma_2(w)$ maps Σ onto Σ and is one-to-one.

(2) For all w and v in SL(2,R),

$$\gamma_2(w)\circ\gamma_2(v)=\gamma_2(wv)\,. \tag{3.18}$$

$$(3)\,f^{-2}(d\mathscr{E}\otimes d\mathscr{E}^*) \tag{3.19}$$

is invariant under $\gamma_2(w)$.

Corollary: The colliding wave condition $k=l=1$ is preserved by $\gamma_2(w)$.

We now have two realizations of SL(2,R); viz., $\gamma_1(w)$ and $\gamma_2(w)$. The key idea of Geroch, when expressed in the language of our SL(2,R) realizations, was to construct a new group by alternate applications of $\gamma_1(v)$ and $\gamma_2(w)$ with different choices of v and w in successive transformations. This creates a nontrivial infinite-dimensional group.

D. The realizations $G_0(\Sigma)$ and $G_0(\Sigma_1)$ of the Geroch group

Definition: Let $G_0(\Sigma)$ denote the set of all compositions of the form

$$\gamma_{r_m}(w_m)\circ\cdots\circ\gamma_{r_1}(w_1)$$

for all choices of $m\geqslant 1$, the SL(2,R) members $w_1,\ldots,w_m$ and the subscript values $r_1,r_2,\ldots,r_m=1$ or 2 (taken in any order).

The following theorem is an immediate consequence of the ones presented in Secs. III B and III C.

Theorem: $G_0(\Sigma)$ is a group of one-to-one mappings of Σ onto Σ.

Definition: Let Σ_1 denote the set of all members of Σ that satisfy the colliding wave condition $k=l=1$ as defined by Eqs. (2.23).

Definition: Let $G_0(\Sigma_1)$ be the set of restrictions to Σ_1 of all members of $G_0(\Sigma)$.

It follows from the preceding theorem and the corollaries in Secs. III B and III C that $G_0(\Sigma_1)$ is a group of one-to-one mappings of Σ_1 onto Σ_1.

E. An example of the generation of a new colliding wave solution by employing members of $G_0(\Sigma_1)$

We shall start with the Nutku–Halil solution. The Ernst potential $E^{\mathrm{NH}}=E_0$ was given by Eq. (2.34) and $\mathscr{E}^{\mathrm{NH}}$ is given by

$$\mathscr{E}_0=XY-2(pY-iqX-xY)(pX-iqY)^{-1}\,, \tag{3.20}$$

where x, y, X, Y are defined by Eqs. (2.32) and (2.41). We want to obtain

$$(E_2,\mathscr{E}_2):=\gamma_2(\epsilon)\circ\gamma_2(w_\Delta)\circ\gamma_1(w)(E_0,\mathscr{E}_0)\,, \tag{3.21}$$

where w_Δ and ϵ are defined by Eqs. (3.8), and w is any member of SO(2,R), which we parametrize as follows:

$$w=\begin{pmatrix}\cos(\nu'/2) & \sin(\nu'/2)\\ -\sin(\nu'/2) & \cos(\nu'/2)\end{pmatrix}. \tag{3.22}$$

Let

$$(E_0',\mathscr{E}_0'):=\gamma_1(w)(E_0,\mathscr{E}_0)\,. \tag{3.23}$$

Then Eqs. (3.4), (3.7), and (3.22) yield

$$E_0'=\gamma_1(w)E_0=(1-\xi')(1+\xi')^{-1}\,, \tag{3.24}$$

where

$$\xi' := (p' - iq')\xi$$

and

$$p' := \cos\nu', \quad q' := \sin\nu' . \tag{3.25}$$

The corresponding $\mathscr{E}$ potential is

$$\begin{aligned}\mathscr{E}_0' &= \gamma_1(w)\mathscr{E}_0 \\ &= XY - 2[pY - iqX - (p'x - iq'y)Y] \\ &\quad \times (pX - iqY)^{-1} .\end{aligned} \tag{3.26}$$

We shall comment on the mode of calculation later.

Next, from Eq. (3.17a) we obtain

$$\gamma_2(w_\Delta)(E_0', \mathscr{E}_0') = (E_0', \mathscr{E}_0' + i\Delta) , \tag{3.27}$$

where E_0' and $\mathscr{E}_0'$ are given by Eqs. (3.24)–(3.26). It is easy to see that $\gamma_2(w_\Delta)E_0' = E_0'$ since adding an imaginary constant to $\mathscr{E}_0'$ does not alter the metric components. That does not mean, however, that this imaginary constant will not show up in the metric after further transformations. In fact, from Eqs. (3.17b) and (3.18),

$$\begin{aligned}\gamma_2(\epsilon)(E_0', \mathscr{E}_0' + i\Delta) &= (\gamma_2(\epsilon)E_0', (\mathscr{E}_0' + i\Delta)^{-1}) \\ &= (E_2, \mathscr{E}_2) ,\end{aligned} \tag{3.28}$$

where we have combined (3.24), (3.27), and (3.28) to give us $(E_2, \mathscr{E}_2)$ as defined by Eq. (3.21). The computation of $E_2 = \gamma_2(\epsilon)E_0'$ is not trivial. The result is

$$E_2 = AB^{-1} , \tag{3.29}$$

where

$$B = (p' + iq') - (px + iqy) , \tag{3.30}$$

$$\begin{aligned}A = &- B\rho^2 + 2[(p' - 2px + p'x^2)Y^2 \\ &+ i(q' - 2qy + q'y^2)X^2] \\ &+ 2i\Delta[py(x^2 - 2) + iqx(y^2 - 2) + xy(p' + iq')] \\ &+ \Delta^2(p' + iq' + px + iqy) .\end{aligned} \tag{3.31}$$

When $\Delta = 0$, $q' = 0$, and $p' = 1$, the above result reduces to the solution given by Eqs. (3.7)–(3.9) in paper I. When $\Delta = 0$, the result reduces to the $n = 2$ solution given by Eqs. (2.37)–(2.41) in the present paper.

For $\Delta = 0$, $q' = 0$, and $p' = 1$, we computed the results given above by several means, including direct integration, as in Eqs. (3.5) and (3.16). However, to obtain the solution with all parameters, we employed a more powerful and efficient method which involves solving a homogeneous Riemann–Hilbert problem to effect the transformation $(E_0, \mathscr{E}_0) \to (E_0', \mathscr{E}_0')$. This method will be detailed in a subsequent paper.

From the A and B given by Eqs. (3.30) and (3.31), both g_{ab} and g_{uv} can be computed by simple algebraic means with the aid of equations given by Ernst.[19] Also, one can employ Eqs. (3.7) and (3.9) in paper I.

Of course, g_{ab} can always be algebraically computed from E by using the definition (2.10) of E.

As regards the computation of g_{uv}, we shall now see that there is a striking shortcut that is generally applicable to the transformation of a metric induced by $\gamma_r(w)$ for any w in SL(2,R).

F. The transformations of g_{uv} induced by $\gamma_1(w)$ and $\gamma_2(w)$

First consider $\gamma_1(w)$. Since Eq. (3.11) implies that $|E_u|^2F^{-2}$ and $|E_v|^2F^{-2}$ are invariant under $\gamma_1(w)$, Eqs. (2.13) and (2.14) imply that

$$g_{uv}' = g_{uv} , \tag{3.32}$$

where $(E', \mathscr{E}') = \gamma_1(w)(E, \mathscr{E})$. This is to be expected, since $E \to \gamma_1(w)E$ is equivalent to an SL(2,R) transformation of the ignorable coordinates.

Consider $\gamma_2(w)$. In this case, it is $|E_u|^2 f^{-2}$ and $|\mathscr{E}_v|^2 f^{-2}$ that are invariant, since $\mathscr{E} \to \gamma_2(w)\mathscr{E}$. Hence, from Eqs. (2.17) and (2.18),

$$g_{22}' g_{uv}' = g_{22} g_{uv} , \tag{3.33}$$

where $(E', \mathscr{E}') = \gamma_2(w)(E, \mathscr{E})$.

G. Some interesting relations involving $\gamma_1(\epsilon)$ and $\gamma_2(\epsilon)$

For the Kasner metrics of index n,

$$E = E_n = \rho^n, \quad \mathscr{E} = \mathscr{E}_n = -\rho^{1-n} . \tag{3.34}$$

Therefore

$$\begin{aligned}&\gamma_1(\epsilon)(E_n, \mathscr{E}_n) = (E_{-n}, \mathscr{E}_{-n}) , \\ &\gamma_2(\epsilon)(E_n, \mathscr{E}_n) = (E_{-n+2}, \mathscr{E}_{-n+2}) , \\ &\gamma_2(\epsilon) \circ \gamma_1(\epsilon)(E_n, \mathscr{E}_n) = (E_{n+2}, \mathscr{E}_{n+2}) .\end{aligned} \tag{3.35}$$

The interesting thing about the above relations is that they essentially carry over to other families of metrics that are obtained by applying a significant class of Kinnersley–Chitre transformations to the Kasner metrics.

For example, consider the family given by Eqs. (2.37)–(2.41). From Eqs. (2.39) and (2.40),

$$\begin{aligned}&T(-n, \nu, \nu' + \pi) = T(n, \nu, \nu') , \\ &T(n, \nu, \nu' \pm 2\pi) = T(n, \nu, \nu') , \\ &T(n, \nu + \pi, \nu' + \pi) = -T(n, \nu, \nu') .\end{aligned} \tag{3.36}$$

Therefore, from Eqs. (2.37) and (2.38),

$$\begin{aligned}&\gamma_1(\epsilon)(E(n, \nu, \nu'), \mathscr{E}(n, \nu, \nu')) \\ &\quad = (E(-n, \nu + \pi, \nu'), \mathscr{E}(-n, \nu + \pi, \nu')) ,\end{aligned} \tag{3.37a}$$

$$\begin{aligned}&\gamma_2(\epsilon)(E(n, \nu, \nu'), \mathscr{E}(n, \nu, \nu')) \\ &\quad = (E(-n + 2, \nu, \nu' + \pi), \mathscr{E}(-n + 2, \nu, \nu' + \pi)) ,\end{aligned} \tag{3.37b}$$

$$\begin{aligned}&\gamma_2(\epsilon) \circ \gamma_1(\epsilon)(E(n, \nu, \nu'), \mathscr{E}(n, \nu, \nu')) \\ &\quad = (E(n + 2, \nu, \nu'), \mathscr{E}(n + 2, \nu, \nu')) .\end{aligned} \tag{3.37c}$$

The general theory behind these remarkable results will be given in a subsequent paper.

IV. AUGMENTATION OF THE GEROCH GROUP BY THE KRAMER–NEUGEBAUER INVOLUTION

A. The augmented Geroch group realization $G_1(\Sigma)$

The set $G_0(\Sigma)$ does not contain two obvious idempotent mappings of Σ onto Σ which we shall denote by γ_{cc} and γ_{KN} and which are defined by

$$\gamma_{cc}(E,\mathscr{E}) := (E^*,\mathscr{E}^*),$$
$$\gamma_{KN}(E,\mathscr{E}) := (-\mathscr{E}^*,-E^*). \tag{4.1}$$

Note that $(\gamma_{cc})^2 = (\gamma_{KN})^2$ is the identity mapping on Σ, and

$$\gamma_{cc}\circ\gamma_{KN}(E,\mathscr{E}) = (-\mathscr{E},-E).$$

Here γ_{KN} will be called the *Kramer–Neugebauer involution* and it is central to the discussion in Sec. IV.

Definition: $G_1(\Sigma)$ will denote the group of all compositions

$$f_m\circ\cdots\circ f_1,$$

for all $m\geqslant 1$, such that $f_1,\ldots,f_m$ are any members of

$$G_0(\Sigma)\cup\{\gamma_{cc},\gamma_{KN}\}.$$

Since Eqs. (2.2) imply that *the colliding wave condition* $k=l=1$ *is preserved by both* γ_{cc} *and* γ_{KN}, we obtain the following theorem.

Theorem: γ_{cc} and γ_{KN} map Σ_1 onto Σ_1; i.e., $G_1(\Sigma_1)$ is a group of one-to-one mappings Σ_1 onto Σ_1.

B. The transformation of g_{uv} induced by γ_{KN}

A relation we shall now derive supplies the new g_{uv} resulting from a Kramer–Neugebauer involution *in terms of the old* g_{22} *and* g_{uv}. Thus it resembles Eq. (3.33), which does the same for the transformation $\gamma_2(w)$.

We start with Eqs. (2.21), from which we derive

$$\frac{1}{u}\left[1-\frac{\rho|\mathscr{E}_u|^2}{4f^2}\right]=\frac{1}{u}\left[1-\frac{\rho|E_u|^2}{4F^2}\right]-\frac{u}{\rho}-\frac{F_u}{F}. \tag{4.2}$$

From Eqs. (2.17), (2.18), and (4.2) we obtain

$$(g'_{22})^{1/2}g'_{uv} = (g_{22})^{1/2}g_{uv}, \tag{4.3}$$

where $(E',\mathscr{E}') = \gamma_{KN}(E,\mathscr{E})$. However, $g'_{22} = \rho(g_{22})^{-1}$. Therefore

$$g'_{uv} = \rho^{-1/2}g_{22}\,g_{uv}, \tag{4.4}$$

which is our final result.

C. The effects of γ_{KN} on the Kasner index n

From the expressions for E_n and $\mathscr{E}_n$ given by Eqs. (3.34) for the Kasner family and from Eqs. (3.35),

$$\gamma_{KN}(E_n,\mathscr{E}_n) = (E_{-n+1},\mathscr{E}_{-n+1}),$$
$$\gamma_{KN}\circ\gamma_1(\epsilon)(E_n,\mathscr{E}_n) = (E_{n+1},\mathscr{E}_{n+1}). \tag{4.5}$$

This effect on n carries over to other families which are obtained from the Kasner one by Kinnersley–Chitre transformations. As an example, for the family given by Eqs. (2.37)–(2.41), with the aid of Eqs. (3.36) and (3.37) one finds

$$\gamma_{KN}(E(n,\nu,\nu'),\mathscr{E}(n,\nu,\nu')) = (E(-n+1,\nu,\nu'+\pi),\mathscr{E}(-n+1,\nu,\nu'+\pi)),$$
$$\gamma_{KN}\circ\gamma_1(\epsilon)(E(n,\nu,\nu'),\mathscr{E}(n,\nu,\nu')) = (E(n+1,\nu,\nu'),\mathscr{E}(n+1,\nu,\nu')). \tag{4.6}$$

Note that, from Eq. (3.37c),

$$\gamma_2(\epsilon)\circ\gamma_1(\epsilon) = [\gamma_{KN}\circ\gamma_1(\epsilon)]^2. \tag{4.7}$$

The generalization of the above relations for arbitrary Kinnersley–Chitre transformations will be proven in a subsequent paper.

D. A new $n=3$ solution

We shall now apply the transformation $\gamma_{KN}\circ\gamma_1(\epsilon)$ to the $n=2$ solution of Eqs. (3.28)–(3.31). We first compute

$$\gamma_1(\epsilon)(E_2,\mathscr{E}_2) = (E_2^{-1},\gamma_1(\epsilon)\mathscr{E}_2), \tag{4.8}$$

where E_2 was given explicitly by Eqs. (3.29)–(3.31), and

$$\mathscr{E}_2 = (\mathscr{E}'_0 + i\Delta)^{-1}, \tag{4.9}$$

where $\mathscr{E}'_0$ was given explicitly by Eq. (3.26). The result for $\gamma_1(\epsilon)\mathscr{E}_2$, i.e., for the second member of the right-hand side of Eq. (4.8), was obtained from the solution of a homogeneous Riemann–Hilbert problem and is given by

$$\begin{aligned}\gamma_1(\epsilon)\mathscr{E}_2 &= -4z^2\rho-\rho^3+(4-i\Delta\rho)(\rho-i\Delta)\\ &\quad + AB^{-1}\{[2(\rho-i\Delta)^3(pY+iqX+p'xY+iq'yX)\\ &\quad + 8z\rho(\rho-i\Delta)(p'yX+iq'xY)](pX+iqY)^{-1}\\ &\quad - 4z^2\rho^2-4(\rho-i\Delta)^2\},\end{aligned} \tag{4.10}$$

where B and A are given explicitly by Eqs. (3.30) and (3.31), and

$$p^2+q^2 = p'^2+q'^2 = 1.$$

Next we apply γ_{KN} to obtain

$$(E_3,\mathscr{E}_3) := \gamma_{KN}\circ\gamma_1(\epsilon)(E_2,\mathscr{E}_2), \tag{4.11}$$

where

$$E_3 = -[\gamma_1(\epsilon)\mathscr{E}_2]^*, \tag{4.12}$$

$$\mathscr{E}_3 = -[AB^{-1}]^*; \tag{4.13}$$

and $\gamma_1(\epsilon)\mathscr{E}_2$ is given by Eq. (4.10), while A and B are given by Eqs. (3.31) and (3.30).

V. FUTURE DEVELOPMENTS

Even when other more elementary methods suffice in principle, we have often found it convenient to solve a homogeneous Hilbert problem[14] (HHP) instead. In the next paper of this series we shall present the formulation of the HHP that we have utilized in deriving new colliding wave solutions. In particular, we shall provide a detailed derivation of our three-parameter generalization of the Ferrari–Ibañez–Bruni two-parameter family of solutions. The HHP is certainly an important piece of artillery to have in one's arsenal as one attempts to enlarge further the family of known colliding wave solutions of the Einstein equations.

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The generalized Weyl correspondence and time-dependent stochastic processes

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The definition and some general properties of the generalized Weyl correspondence between stochastic processes and operator-valued real functions on a Hilbert space plus a trace class operator are given. The relation between the derivatives of an operator-valued function and the derivative of the corresponding stochastic process are studied. When the operator-valued function is the position (or momentum) in the Heisenberg picture, a condition for the positivity of the joint distribution functions of the corresponding process is given, provided that the evolution Hamiltonian be quadratic in the position and momentum. Finally, the case of an arbitrary Hamiltonian evolution for the position operator is studied and the two-dimensional density functions of the process is related to the Wigner function associated to some state $\hat{\rho}$, and a necessary condition for the positivity of the densities is given.

I. INTRODUCTION

The idea of a generalized Weyl correspondence (GWC) has already been presented in previous papers.[1-3] This correspondence shows a relation between random variables and linear operators on a separable Hilbert space $\mathscr{H}$ as well as between signed measures on a certain sample space and trace class operators on $\mathscr{H}$. We here recall its definition.

Let $(X_j)_{j\in J}$ be a set of real random variables and $(\hat{x}_j)_{j\in J}$ a set of linear operators on $\mathscr{H}$, where J is an arbitrary index set. If there exists a trace class operator $\hat{\rho}$ such that for any finite set of indices $\{j_i,...,j_n\}\subset J$ and any real numbers $\alpha_{j_1},...,\alpha_{j_n}$,

$$E\{\exp[i(\alpha_{j_1}X_{j_1}+\cdots+\alpha_{j_n}x_{j_n})]\} = \mathrm{tr}\{\hat{\rho}\exp[i(\alpha_{j_1}\hat{x}_{j_1}+\cdots+\alpha_{j_n}\hat{x}_{j_n})]\} \quad (1)$$

holds, then we say that there exists a GWC between the random variables and the operators. Here $E\{\cdots\}$ means expectation value. Each of the random variables acts on a sample space Ω which is endowed with a finite measure such that $\mu(\Omega)=1$. Here μ is not necessarily non-negative [i.e., there may exist a measurable set $A\subset\Omega$ such that $\mu(A)<0$]. Usually, Ω will be the Cartesian product of the ranges of the variables $(X_j)_{j\in J}$ and X_j the projection of Ω on its jth coordinate, although this construction of Ω is not always necessary.

References 1–3 deal with the general properties of this GWC as well as with particular examples. On the other hand, it is a generalization of the classical Weyl correspondence (CWC) which assigns a Hermitian operator to a real function of the coordinates of the position Q and the momentum P in phase space.[4-6] Here Q and P have the role of the random variables X_j. The CWC also assigns a finite measure on the phase space to any quantum state (positive operator on $\mathscr{H}$ with trace 1). As in the general case, this measure is not non-negative in general. Here, the index set J contains $2N$ elements, where N is the dimension of the configuration space.

A stochastic process is a set of random variables.[7] Usually, this set is indexed by an interval J of the real line which eventually is the whole real line R. For any $t\in J$, we have a random variable we call $X(t)$. Here $X(t)$ is a measurable mapping from a certain sample space Ω into R.

To adapt the original definition of GWC to this particular case is now simple. Let $\hat{x}(t)$ be a set of linear operators on $\mathscr{H}$, where $t\in J$. Here $X(t)$ and $\hat{x}(t)$ are related through a GWC if there exists a trace operator $\hat{\rho}$ on $\mathscr{H}$ and a signed measure μ on Ω such that

$$E\{\exp[i(\alpha_1X(t_1)+\cdots+\alpha_nX(t_n))]\} = \int_\Omega \exp[i(\alpha_1X(t_1)+\cdots+\alpha_nX(t_n))]d\mu = \mathrm{tr}\{\hat{\rho}\exp[i(\alpha_1\hat{x}(t_1)+\cdots+\alpha_n\hat{x}(t_n))]\} \quad (2)$$

for any finite set of times $\{t_1,...,t_n\}$ and whatever real numbers of $\alpha_1,...,\alpha_n$, where n is also arbitrary.

We define a stochastic vector as an N-dimensional vector whose components are stochastic processes. For any $t\in J$, $(X_1(t),...,X_N(t))$ is a measurable mapping from Ω onto a subset of R^N.

A stochastic field is a further generalization of a stochastic process. Let A be any set. A stochastic field is a set of stochastic proceses indexed by A. In particular, a stochastic vector is a stochastic field with $A=\{1,2,...,N\}$ and a stochastic process is also a stochastic field with $A=\{\phi\}$ (or any set containing one element only). The denomination of a stochastic field is properly used when $A\subset R^3$. Then the mapping $a\to X(t,a)$ assigns a stochastic processs to any point of the region A which is the physical space in which the phenomenon described by the stochastic field $X(t,a)$, $a\in A$, occurs.

For a stochastic process $X(t)$, we define the finite-di-

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mensional distribution function as

$$F(x_1,t_1) = \mu\{X(t_1) \leqslant x_1\},$$
$$\vdots \tag{3}$$
$$F(x_1 t_1;\cdots;x_n,t_n) = \mu\{X(t_1) \leqslant x_1;\ldots;X(t_n) \leqslant x_n\},$$

for all $t_1,t_2,\ldots,t_n$ in J, and the joint densities as

$$\rho(x_1,t_1) = \frac{\partial F(x_1,t_1)}{\partial x_1},$$
$$\vdots \tag{4}$$
$$\rho(x_1,t_1;\ldots;x_n,t_n) = \frac{\partial^n F(x_1,t_1;\ldots;t_n,t_n)}{\partial x_1 \cdots \partial x_n}.$$

The partial derivatives in (4) should be understood in the sense of the derivatives of distributions, which coincides with the usual sense of the derivative when the finite-dimensional distribution functions are absolutely continuous. If μ is a *positive* probability measure all the distribution functions are non-negative.

The finite-dimensional distribution functions do not fix the process $X(t)$ uniquely. There are many examples of two different stochastic processes having the same finite-dimensional distribution functions.

Let us go back to Eq. (2). It can be written as

$$\int_{R^n} \exp\{i(\alpha_i x_1 + \cdots + \alpha_n x_n)\} \times \rho(x_1,t_1;\ldots;x_n,t_n)\,dx_1 \cdots dx_n = \mathrm{tr}\{\hat{\rho}\exp[i(\alpha_1 \hat{x}(t_1) + \cdots + \alpha_n \hat{x}(t_n))]\}, \tag{5}$$

whence

$$\rho(x_1,t_1;\ldots;x_n,t_n) = \frac{1}{(2\pi)^n}\int_{R^n} \exp\{-i(\alpha_1 x_1 + \cdots + \alpha_n x_n)\} \times \mathrm{tr}\{\hat{\rho}\exp[i(\alpha_1 \hat{x}(t_1) + \cdots + \alpha_n \hat{x}(t_n))]\} \times d\alpha_1 \cdots d\alpha_n. \tag{6}$$

Equation (6) is a consequence of the properties of the Fourier transform, and gives us the following information: Since the finite-dimensional distribution functions and hence their corresponding densities do not fix a process uniquely, in general we shall have more than one process associated to the set of operators $\hat{x}(t)$ and $\hat{\rho}$ through a GWC.

If we have a stochastic vector, the measure μ on Ω determines the following distribution functions:

$$F(x_{11},\ldots,x_{N1},t_1;\ldots;x_{1s},\ldots,x_{Ns},t_s) = \mu\{X_1(t_1) \leqslant x_{11},\ldots,X_N(t_1) \leqslant x_{N1};\ldots;X_1(t_s) \leqslant x_{1s},\ldots,X_N(t_s) \leqslant x_{Ns}\} \tag{7}$$

and the corresponding densities:

$$\rho(x_{11},\ldots,x_{N1}\,t_1;\ldots;x_{1s};\ldots;x_{Ns},t_s) = \frac{\partial^{s\times N} F(x_{11},\ldots,x_{Ns})}{\partial x_{11}\cdots\partial x_{Ns}}.$$

The definition of GWC can also be used to associate stochastic vectors to operator-valued real functions with N components, as for example the position or momentum operators on $L^2(R^N)$ in the Heisenberg picture. Let $\overline{X}(t) = (X_1(t),\ldots,X_N(t))$ be a stochastic vector and $\bar{\hat{x}}(t) = (\hat{x}_1(t),\ldots,\hat{x}_N(t))$ be an N-dimensional operator-valued real function, where t runs over an interval J of the real line. Here $\overline{X}(t)$ and $\bar{\hat{x}}(t)$ are related through the GWC if there exists a signed measure μ on Ω with $\mu(\Omega) = 1$ and a trace class operator $\hat{\rho}$ on $\mathscr{H}$ such that

$$E\{\exp[i(\alpha_{11}X_1(t_1) + \cdots + \alpha_{N1}X_n(t_1) + \cdots + \alpha_{1s}X_1(t_s) + \cdots + \alpha_{Ns}X_N(t_s))]\} = \int_{R_{N\times s}} \exp[i(\alpha_{11}x_{11} + \cdots + \alpha_{N1}x_{N1} + \cdots + \alpha_{1s}x_{1s} + \cdots + \alpha_{Ns}x_{Ns})], \tag{8}$$

$$\int \rho(x_{11},\ldots,x_{N1},t_1;\ldots;x_{1s},\ldots,x_{Ns},t_s)\,dx_{11}\cdots dx_{Ns} = \mathrm{tr}\{\hat{\rho}\exp[i(\alpha_{11}\hat{x}_1(t_1) + \cdots + \alpha_{N1}\hat{x}_N(t_1) + \cdots + \alpha_{1s}\hat{x}_1(t_s) + \cdots + \alpha_{Ns}\hat{x}_N(t_s))]\} \tag{9}$$

for any $\{t_1,\ldots,t_s\} \subset J$ and any real numbers $\alpha_{11},\ldots,\alpha_{Ns}$.

From (9), it follows that

$$\rho(x_{11},\ldots,x_{N1},t_1;\ldots;x_{1s},\ldots,x_{Ns},t_s) = \frac{1}{(2\pi)^{N\times s}}\int_{R^{N\times s}} d\alpha_{11}\cdots d\alpha_{Ns} \times \exp\{-i(\alpha_{11}x_{11} + \cdots + \alpha_{Ns}x_{Ns}) + \mathrm{tr}\{\hat{\rho}\exp[i(\alpha_{11}\hat{x}_1(t_1) + \cdots + \alpha_{Ns}\hat{x}_N(t_s))]\}. \tag{10}$$

The present paper contains three main sections. In Sec. II, we study the relation between the derivative of the process and the derivative of the operator-valued function $\hat{x}(t)$. Section III starts with a one-dimensional problem. Here, $\hat{x}(t)$ is the position operator of a particle on the Heisenberg picture. The time evolution of $\hat{x}(t)$ is controlled by a quadratic time independent Hamiltonian. In this case, the density function of each of the random variables in the process $X(t)$ can be interpreted as the classical probability density of finding the particle in the configuration space at the time t, provided that all the joint densities of the process are positive. We give a sufficient condition for this positivity: The Wigner function of $\hat{\rho}$ must be positive at $t = 0$. This result is easily generalized to the case of N dimensions. In Sec. IV, we discuss a necessary condition for the positivity of μ when $\hat{\rho}$ is a pure state and we are in the situation described in Sec. II.

II. GENERAL CONSIDERATIONS

We start with the assumption of the existence of a GWC for a stochastic process $X(t)$ or a stochastic vector $(X_1(t),\ldots,X_n(t))$. This means that Eqs. (2) and (9) make sense and, in particular, their right-hand sides are well defined, which in (2) happens if $\exp\{i(\alpha_i\hat{x}(t_1) + \cdots + \alpha_n\hat{x}(t_n))\}$ is a bounded operator for all the α_i and all the values of the time parameter. There are two interesting situations in which this occurs: (1) all the $\hat{x}(t)$ are bounded for all $t \in J$, and (2) all the operators of the form $\alpha_1\hat{x}(t_1) + \cdots + \alpha_n\hat{x}(t_n)$ are essentially self-adjoint on a common domain dense in $\mathscr{H}$. This occurs, in particular, when $\hat{x}(t) = h(t)\hat{x}(0) + g(t)\hat{p}(0) + \eta(t)I$, where $\hat{x}(0)$ and $\hat{p}(0)$ are, respectively, the position and momentum operators in one dimension, I is the identity operator, and $h(t)$,

$g(t)$, and $\eta(t)$ are real functions. This case and its generalizations to N dimensions is studied in this paper.

In order to simplify our notation, we mainly deal here with stochastic processes $X(t)$. However, most of our results are trivially extensible to stochastic vectors.

We can look at the random variable $X(t_0)$ for each $t_0 \in J$ in two ways. First, $X(t_0)$ can be properly considered as something which "transports" measure from Ω to R. Under this point of view, what really matters of $X(t_0)$ is its probability distribution and its joint distributions with the other random variables in the process. The other possibility is to look at $X(t_0)$ as a measurable function from Ω into R. Both points of view are quite different, since the first one depends critically on the measure μ on Ω while the second is independent on μ. To visualize the difference, one can imagine a situation in which $X(t) = X(0)$ $\forall t \in J$ in measure (this means that $\mu\{w/[X(t)](w) \neq [X(0)](w)$ for some $t \in J\} = 0$ if μ is positive; if μ is not positive and $\mu = \mu_1 - \mu_2$ is the Jordan decomposition of μ, we have to require that $\mu_i\{w/[X(t)](w) \neq [X(0)](w)$, for some $t \in J\} = 0$ with $i = 1,2$) and the measurable functions are all different. Such a process can be easily constructed.[8]

Henceforth, a stochastic process will be a set of measurable functions $X(t)$ on a sample space Ω; where t belongs to an open interval J of the real line; plus a bounded signed measure μ on Ω with $\mu(\Omega) = 1$ (a signed measure is bounded if $\mu = \mu_1 - \mu_2$, where μ_1 and μ_2 are positive and finite). If μ is a probability measure, we say that the process is veritable. All the finite-dimensional distribution functions and their corresponding densities are well defined provided the boundedness of μ. A process is veritable if and only if all the densities are positive (a.e. with respect to the Lebesgue measure).

The stochastic relation among the $X(t)$ can appear in many other ways. An interesting case arises when the identity $X(t) = h_1(t)X_1 + \cdots + h_n(t)X_n$ holds in measure, where $h_1(t),\ldots,h_n(t)$ are real functions on J and $X_1,\ldots,X_n$ are n random variables on Ω. The interest of this kind of process will be evident later.

For any $t \in J$, the GWC maps $X(t)$, considered as a measurable function on Ω, into $\hat{x}(t)$, provided that certain conditions are satisfied.[1,2] Assume now that $X(t)$ and $\hat{x}(t)$ admit a derivative with respect to t in some sense. Are these derivatives related through a GWC? If the derivative for $\hat{x}(t)$ exists at some point, does it for $X(t)$ and vice versa? Our next objective is to give an answer to these questions. In order to make our procedures and results comprehensible to a wide audience, we start with the basic definitions.

III. DEFINITIONS

(1) Let $X(t)$ be a veritable stochastic process. If all the second moments existed, we define a norm for the random variables in the process as

$$\|X(t)\| = \{E\{X^2(t)\}\}^{1/2} = \left\{\int_\Omega X^2(t)d\mu\right\}^{1/2}. \quad (11)$$

If $X(t)$ were not veritable, we still could define a norm for each of the random variables $X(t)$, provided that their second moments existed with respect to the measures μ_1 and μ_2, where $\mu = \mu_1 - \mu_2$ is the Jordan decomposition of μ. The square of this norm is given by

$$\|X(t)\|^2 = \int_\Omega X^2(t)d\mu_1 + \int_\Omega X^2(t)d\mu_2 \quad (12)$$

and the second moment of $X(t)$ with respect to μ is

$$E\{X^2(t)\} = \int_\Omega X^2(t)d\mu_1 - \int_\Omega X^2(t)d\mu_2 = \int_\Omega X^2(t)d\mu. \quad (13)$$

In the two cases considered here, we have that $E\{X(t)X(t')\} < \infty$ for any $t,t' \in J$ and

$$E\{X^2(t)\} = -\frac{d^2}{d\alpha^2} E\{e^{i\alpha X(t)}\}|_{\alpha=0}. \quad (14)$$

(2) $X(t)$ is continuous at $t = t_0$ if $\|X(t) - X(t_0)\| \to 0$ when $t \to t_0$. Here $X(t)$ is continuous if it is so at any $t \in J$.

(3) $X(t)$ admits a derivative at t_0 if there exists a random variable $\dot{X}(t_0)$ with finite second moment such that

$$\lim_{s\to 0}\|[X(t_0+s) - X(t_0)]/s - \dot{X}(t_0)\| = 0.$$

If $X(t)$ admits a derivative at any $t \in J$, we have a stochastic process $\dot{X}(t)$ that we call the derivative of $X(t)$.

Definitions (2) and (3) are independent of whether the process is veritable or not.

(4) Let $Y(t,s)$ be a collection of stochastic processes indexed by a continuous real index s. A process $X(t)$ is the limit of $Y(t,s)$ when s goes to zero if

$$\lim_{s\to 0}\|Y(t,s) - X(t)\| = 0. \quad (15)$$

If all the $Y(t,s)$ are veritable, its limit $X(t)$ is also veritable. In this case, the joint characteristic function

$$E\{\exp(\{\alpha_1 Y(t_1,s) + \cdots + \alpha_n Y(t_n,s)\})\} = \varphi_{s,t_1,\ldots,t_n}(\alpha_1,\ldots,\alpha_n) \quad (16)$$

converges pointwise to the characteristic function

$$E\{\exp(i\{\alpha_1 X(t_1) + \cdots + \alpha_n X(t_n)\})\}. \quad (17)$$

This result is also true even if the $Y(t,s)$ were not veritable.

(5) Now assume that all the operators in the family $\hat{x}(t)$ are defined in a common domain $\mathscr{D}$ dense in the Hilbert space $\mathscr{H}$. Here $\hat{x}(t)$ admits a *strong derivative* or simply a derivative at $t_0 \in J$ if there exists a linear mapping $\dot{\hat{x}}(t_0)$ from $\mathscr{D}$ to $\mathscr{H}$ such that

$$\lim_{s\to 0}\|\{[\hat{x}(t_0+s) - \hat{x}(t_0)]/s - \dot{\hat{x}}(t_0)\}\varphi\| = 0 \quad (18)$$

$\forall \varphi \in \mathscr{D}$. In (18) we have used the standard Hilbert space norm. If $\hat{x}(t)$ admits a derivative at any $t \in J$, we say that it is derivable.

When all the $\hat{x}(t)$ are bounded and there is a bounded operator $\dot{\hat{x}}(t_0)$ such that in the norm operator sense

$$\lim_{s\to 0}\|[\hat{x}(t_0+s) - \hat{x}(t_0)]/s - \dot{\hat{x}}(t_0)\| = 0, \quad (19)$$

we say that $\dot{\hat{x}}(t_0)$ is the *uniform derivative* of $x(t)$ at t_0. The existence of the uniform derivative implies that of the derivative but the converse is not true.

Definitions (1)–(5) are standard and appear in the textbooks.[9–12]

Our next goal is to prove that, under certain conditions, if $X(t)$ and $\hat{x}(t)$ are related through a GWC so are their derivatives. Henceforth, we shall assume that for any $t\in J$ the operators $\hat{x}(t)$ and $\dot{\hat{x}}(t)$ and their linear combinations are essentially self-adjoint on a common domain $\mathscr{D}$ dense in $\mathscr{H}$. In this case $\exp\{i(\alpha_1\hat{x}(t_1)+\cdots+\alpha_n\hat{x}(t_n))\}$ and $\exp\{i(\alpha_1\dot{\hat{x}}(t_1)+\cdots+\alpha_n\dot{\hat{x}}(t_n))\}$ are well defined unitary operators on $\mathscr{H}$ for any real values of $\alpha_1,\ldots,\alpha_n$ and arbitrary $t_1,\ldots,t_n$ in J. For our purpose, we need to begin with some results in functional analysis.

Theorem I: Let $\{A_n\}_{n\in N}, A$ be self-adjoint operators and $\mathscr{D}$ a common core for them. If $A_n\to A$ for any $\varphi\in\mathscr{D}$, then $e^{itA_n}\varphi\to e^{itA}\varphi$, $\forall\varphi\in\mathscr{H}$ and $\forall t\in R$.

The proof can be seen in Ref. 12.

Corollary I: Assume that $\forall\varphi\in\mathscr{D}$,

$$\{\alpha_1\hat{x}(t_1+s)+\cdots+\alpha_n\hat{x}(t_n+s)\}\varphi \to\{\alpha_1\hat{x}(t_1)+\cdots+\alpha_n\hat{x}(t_n)\}\varphi, \tag{20}$$

wherever $s\to 0$ $\forall\varphi\in\mathscr{D}$. Then

$$\exp(i\{\alpha_1\hat{x}(t_1+s)+\alpha_n\hat{x}(t_n+s)\})\varphi \to\exp(i\{\alpha_1\hat{x}(t_1)+\cdots+\alpha_n\hat{x}(t_n)\})\varphi \tag{21}$$

$\forall\varphi\in\mathscr{H}$ and any $\alpha_1,\ldots,\alpha_n$ in R.

Corollary II:

$$\lim_{s\to 0}\exp\left(i\left\{\alpha_1\left[\frac{\hat{x}(t_1+s)-\hat{x}(t_1)}{s}\right]+\cdots+\alpha_n\left[\frac{\hat{x}(t_n+s)-\hat{x}(t_n)}{s}\right]\right\}\right)\varphi=\exp(i\{\alpha_1\dot{\hat{x}}(t_1)+\cdots+\alpha_n\dot{\hat{x}}(t_n)\})\varphi. \tag{22}$$

Corollary III: Assume that $\hat{\rho}$ is a trace class normal operator (in particular $\hat{\rho}$ can be positive). Then

$$\lim_{s\to 0}\mathrm{tr}\left\{\hat{\rho}\exp\left(i\left\{\alpha_1\left[\frac{\hat{x}(t_1+s)-\hat{x}(t_1)}{s}\right]+\cdots+\alpha_n\left[\frac{\hat{x}(t_n+s)-\hat{x}(t_n)}{s}\right]\right\}\right)\right\}=\mathrm{tr}\{\hat{\rho}\exp(i\{\alpha_1\dot{\hat{x}}(t_1)+\cdots+\alpha_n\dot{\hat{x}}(t_n)\})\}. \tag{23}$$

Proof: Since $\hat{\rho}$ is normal, the following spectral decomposition works[12]:

$$\hat{\rho}=\sum_{k=1}^{\infty}\lambda_k|\psi_k\rangle\langle\psi_k|, \tag{24}$$

where $\hat{\rho}\psi_k=\lambda_k\psi_k$, $\Sigma_{k=1}^{\infty}|\lambda_k|<\infty$, and $\|\psi_k\|=1$. Assume that all the λ_k but a finite number are zero. Then, Corollary III follows from Corollary II trivially. The proof in the general case is a little more involved. In order to simplify the notation, we shall here demonstrate (23) for $n=1$. The case of $n\neq 1$ does not require more sophistication.

Therefore consider

$$\mathrm{tr}\left\{\hat{\rho}\exp\left\{i\alpha\left[\frac{\hat{x}(t+s)-\hat{x}(t)}{s}\right]\right\}\right\} \tag{25}$$

and used $\hat{y}(s)=[\hat{x}(t+s)-\hat{x}(t)]/s$. Thus

$$\mathrm{tr}\{\rho e^{i\alpha\hat{y}(s)}\}=\sum_{k=1}^{\infty}\lambda_k\langle\psi_k|e^{i\alpha\hat{y}(s)}|\psi_k\rangle =\sum_{k=1}^{\infty}f_k(s), \tag{26}$$

$$|f_k(s)|=|\lambda_k|\,|\langle\psi_k|e^{i\alpha\hat{y}(s)}|\psi_k\rangle| \leqslant|\lambda_k|\,\|\psi_k\|\,\|e^{i\alpha\hat{y}(s)}\psi_k\|. \tag{27}$$

Since $\hat{y}(s)$ is self-adjoint and α is a real number, $e^{i\alpha\hat{y}(s)}$ is unitary. Thus $|f_k(s)|\leqslant|\lambda_k|$ and

$$|\mathrm{tr}\{\hat{\rho}e^{i\alpha\hat{y}(s)}\}|\leqslant\sum_{k=1}^{\infty}|f_k(s)|\leqslant\sum_{k=1}^{\infty}|\lambda_k|<\infty. \tag{28}$$

Hence the Weierstrass M criterion[13] says that the series (26) converges uniformly in s. Since

$$\lim_{s\to 0}\langle\psi_k|e^{i\alpha\hat{y}(s)}|\psi_k\rangle=\langle\psi_k|e^{i\alpha\dot{\hat{x}}(t)}|\psi_k\rangle$$

exists for any $k=1,2,\ldots$, the limit of the series exists for $s\to 0$ and is $\mathrm{tr}\{\hat{\rho}\exp\{i\alpha\dot{\hat{x}}(t)\}\}$.

Theorem II: Assume the following.

(a) $X(t)$ is a stochastic process on Ω and μ is a bounded signed measure on Ω.

(b) The derivative $\dot{X}(t)$ exists at each $t\in J$.

(c) $\hat{\rho}$ is a normal trace class operator on $\mathscr{H}$.

(d) The operators $\hat{x}(t)$ and their real linear combinations are e.s.a. on a common domain $\mathscr{D}$ dense in $\mathscr{H}$.

(e) The derivative $\dot{\hat{x}}(t)$ exists for any $t\in J$ and any real linear combination of these operators is e.s.a. on $\mathscr{H}$.

(f) There exists a GWC relating $X(t)$ to $\hat{x}(t)$ and μ to $\hat{\rho}$.

Then, the GWC relates $\dot{X}(t)$ and $\dot{\hat{x}}(t)$ with μ and $\hat{\rho}$ being the same.

Proof: After Corollary III, the following limit is well defined:

$$\lim_{s\to 0} \operatorname{tr}\hat{\rho}\exp i\left\{\alpha_1\frac{x(t_1+s)-x(t_1)}{s}+\cdots+\alpha_n\frac{x(t_n+s)-x(t_n)}{s}\right\}$$
$$=\operatorname{tr}\{\hat{\rho}\exp\{i[\alpha_1\dot{\hat{x}}(t_1)+\cdots+\alpha_n\dot{\hat{x}}(t_n)]\}\}$$
$$=\lim_{s\to 0} E\left\{\exp\left\{i_1\left[\frac{X(t_1+s)-X(t_1)}{s}+\cdots+\alpha_n\frac{X(t_n+s)-X(t_n)}{s}\right]\right\}\right\}, \tag{29}$$

the derivative of $X(t)$ exists by hypothesis. Thus after the comments in Definition 4, this limit is

$$(29)=E\left[\exp[i(\alpha_1\dot{X}(t_1)+\cdots+\alpha_n\dot{X}(t_n))]\right]. \tag{30}$$

The next question we want to answer is if the existence of $\dot{\hat{x}}(t)$ says something about the existence of the derivative of $X(t)$. In the next theorem we do not assume the existence of the moments of $X(t)$.

Theorem III: Assumptions (c)–(f) in Theorem II are also valid here, but $X(t)$ is veritable. Then the functions

$$\lim_{s\to 0} E\left\{\exp\left[i\left(\alpha_1\frac{X(t_1+s)-X(t_1)}{s}+\cdots+\alpha_n\frac{X(t_n+s)-X(t_n)}{s}\right)\right]\right\}=\varphi_{t_1,\ldots,t_n}(\alpha_1,\ldots,\alpha_n) \tag{31}$$

are the characteristic functions of a certain process.

Proof: Since $\hat{\rho}$ is a normal operator, the limit (31) equals to

$$\operatorname{tr}\{\hat{\rho}\exp\{i(\alpha_1\dot{\hat{x}}(t_1)+\cdots+\alpha_n\dot{\hat{x}}(t_n))\}\}=\sum_{k=1}^{\infty}\lambda_k\langle\psi_k|\exp[i(\alpha_1\dot{\hat{x}}(t_1)+\cdots+\alpha_n\dot{\hat{x}}(t_n))]|\psi_k\rangle, \tag{32}$$

where the λ_k are the eigenvalues of $\hat{\rho}$ and the ψ_k their corresponding eigenvectors. If we prove that (32) is continuous on $\overline{\alpha}=(\alpha_1,\ldots,\alpha_n)$, Theorem III would be proved.

The series in (32) converges uniformly on $\overline{\alpha}$. To show this assertion, we use the Weierstrass M criterion as we did it in the proof of Corollary III. Furthermore, we know after the Stone theorem that

$$\langle\psi_k|\exp\{i\{\alpha_1\dot{\hat{x}}(t_1)+\cdots+\alpha_n\dot{\hat{x}}(t_n)\}\}|\psi_k\rangle$$

is continuous on $\overline{\alpha}$. Therefore the series in (32) is continuous on $\overline{\alpha}$, since it is the limit of a sequence of continuous functions on $\overline{\alpha}$ converging uniformly on $\overline{\alpha}$.

This result cannot be extended to the case in which μ is nonpositive. In this case the limit (31) could not be the difference between two characteristic functions.

Obviously, if $X(t)$ is derivable, (31) are the joint characteristic functions of the derivative. However, we cannot claim that we have proved the existence of the derivative of $X(t)$.

Its existence requires a further assumption. We start the discussion with four lemmas.

Lemma I: Assume that we are in the conditions of Theorem III and that any real combination of the form $\alpha_1\hat{x}(t_1)+\cdots+\alpha_n\hat{x}(t_n)+\beta_1\dot{\hat{x}}(t_1)+\cdots+\beta_n\dot{\hat{x}}(t_n)$ is self-adjoint. Then the limit

$$\lim_{s\to 0} E\left[\exp i\left\{\alpha_1 X(t_1)+\beta_1\frac{X(t_1+s)-X(t_1)}{s}+\cdots+\beta_n\frac{X(t_n+s)-X(t_n)}{s}\right\}\right] \tag{33}$$

is well defined and represents the characteristic function of a stochastic vector with two components.

Proof: It is simple to realize that

$$\lim_{s\to 0}\operatorname{tr}\left\{\hat{\rho}\exp i\left\{\alpha_i\hat{x}(t_1)+\beta_1\frac{\hat{x}(t_1+s)-\hat{x}(t_1)}{s}+\cdots+\beta_n\frac{\hat{x}(t_n+s)-\hat{x}(t_n)}{s}\right\}\right\}$$
$$=\operatorname{tr}\{\hat{\rho}\exp i(\alpha_1\hat{x}(t_1)+\beta_1\dot{\hat{x}}(t_1)+\cdots+\alpha_n\hat{x}(t_n)+\beta_n\dot{\hat{x}}(t_n))\} \tag{34}$$

is continuous at zero function of $(\alpha_1,\beta_1,\ldots,\alpha_n,\beta_n)$.

If $X(t)$ admits a derivative, this stochastic vector is $(X(t),\dot{X}(t))$.

Remark: If $(X(t),\pi(t))$ is some stochastic vector having (33) as joint characteristic functions, we can write

$$E\{\exp(i\{\alpha_1X(t_1)+\beta_1\pi(t_1)+\cdots+\alpha_nX(t_n)+\beta_n\pi(t_n)\})\}$$
$$=\operatorname{tr}\{\hat{\rho}\exp i\{\alpha_1\hat{x}(t_1)+\beta_1\dot{\hat{x}}(t_1)+\cdots+\alpha_n\hat{x}(t_n)+\beta_n\dot{\hat{x}}(t_n)\}\}. \tag{35}$$

If for any $t\in J$, $X(t)$, and $\pi(t)$ admitted moments of second order, we would have

$$(1)\quad E\left\{\left(\frac{X(t+s)-X(t)}{s}-\pi(t)\right)^2\right\}, \tag{36}$$

$$(2)\quad -\frac{d^2}{d\alpha^2}E\left\{\exp\left(i\alpha\left[\frac{X(t+s)-X(t)}{s}-\pi(t)\right]\right)\right\}\Big|_{\alpha=0}=E\left\{\left(\frac{X(t+s)-X(t)}{s}-\pi(t)\right)^2\right\}. \tag{37}$$

Lemma II: Let A be a self-adjoint operator and $\hat{\rho}$ a trace class normal operator with $\hat{\rho} = \Sigma_{k=1}^{\infty} \lambda_k |\psi_k\rangle\langle\psi_k|$ with $\psi_k \in \mathscr{D}(A)$, the domain of A. If $\mathrm{tr}\{\hat{\rho}|A|^n\} < \infty$,

$$\frac{d^n}{d\alpha^n} \mathrm{tr}\{\hat{\rho} e^{i\alpha A}\}|_{\alpha=0} = (i)^n \mathrm{tr}\{\hat{\rho} A^n\}. \tag{38}$$

Proof: See Appendix A.

Lemma III: Let $\hat{\rho}$ be as in Lemma II, with ψ_k in the domains of two self-adjoint operator A and B and $B\psi_k \in \mathscr{D}(A)$. If $\mathrm{tr}\{\rho A^2\} < \infty$ and $\mathrm{tr}\{\hat{\rho} B^2\} < \infty$, then $\mathrm{tr}\{\hat{\rho} AB\} < \infty$.

Proof: See Appendix B.

Lemma IV: Under the conditions in Lemma I, if $\mathrm{tr}\{\hat{\rho}\hat{x}^2(t)\}$ and $\mathrm{tr}\{\hat{\rho}\hat{x}^2(t)\}$ are both finite and $\hat{\rho}$ is a normal trace class operator, then

$$\mathrm{tr}\left\{\hat{\rho}\left[\frac{(\hat{x}(t+s)-\hat{x}(t))}{s} - \dot{\hat{x}}(t)\right]^2\right\} \tag{39}$$

for any $t \in J$ and s in a neighborhood of zero.

Proof: It is obvious after Lemmas II and III.

Theorem IV: We are under the conditions of Theorem III and the two following hypothesis: (a) $X(t)$ and $\pi(t)$ (see remark after Lemma I) have finite second moments $\forall t \in J$; and (b) either

$$\hat{\rho} = \sum_{k=1}^{N} \lambda_k |\psi_k\rangle\langle\psi_k|$$

with N finite and the ψ_k belong to proper domains so that Lemmas II and III can be used, or the operators $\hat{x}(t)$ and $\dot{\hat{x}}(t)$ are bounded and the derivative exists in the norm operator sense.

Then, $\dot{X}(t) = \pi(t)$.

Proof: A proper choice of the constants in (35) yields

$$E\left\{\exp\left(i\alpha\left[\frac{X(t+s)-X(t)}{s} - \pi(t)\right]\right)\right\}$$
$$= \mathrm{tr}\left\{\hat{\rho}\exp\left(i\alpha\left[\frac{\hat{x}(t+s)-\hat{x}(t)}{s} - \dot{\hat{x}}(t)\right]\right)\right\}. \tag{40}$$

If we take second derivatives on α at the point $\alpha = 0$, we have

$$E\left\{\left(\frac{X(t+s)-X(t)}{s} - \pi(t)\right)^2\right\}$$
$$= \mathrm{tr}\left\{\hat{\rho}\left[\frac{\hat{x}(t+s)-\hat{x}(t)}{s} - \dot{\hat{x}}(t)\right]^2\right\}. \tag{41}$$

Hypothesis (b) implies that the lhs of (41) has a limit when $s \to 0$ and that this limit is zero. Since the derivative of a process is unique, Theorem IV follows.

Theorem V: We are under the conditions of Theorem IV, but we ignore that $\pi(t)$ have finite second moments.

Then, the derivative of $X(t)$ exists.

Proof: A sufficient condition for the existence of the derivative is the existence of the limit[10]

$$\lim_{s,\tau\to 0} \frac{1}{s\tau}\{E[X(t+s)X(t'+\tau)] - E[X(t+s)X(t')]$$
$$- E[X(t)X(t'+\tau)] + E[X(t)X(t')]\}$$
$$= \lim_{s,\tau\to 0} E\left\{\frac{X(t+s)-X(t)}{s}\,\frac{X(t'+X)-X(t')}{\tau}\right\}. \tag{42}$$

The existence of a GWC between $X(t)$ and $\hat{x}(t)$ implies that

$$E\{\exp(i\alpha\{\alpha_1 X(t_1) + \alpha_2 X(t_2)\})\}$$
$$= \mathrm{tr}\{\hat{\rho}\exp(i\alpha\{\alpha_1\hat{x}(t_1) + \alpha_2\hat{x}(t_2)\})\}, \tag{43}$$

where α, α_1, and α_2 are arbitrary real numbers and t_1, t_2 belong to J.

Deriving twice with respect to α yields

$$E\{(\alpha_1 X(t_1) + \alpha_2 X(t_2))^2\}$$
$$= \alpha_1^2 E(X^2(t_1)) + 2\alpha_1\alpha_2 E(X(t_1)X(t_2))$$
$$+ \alpha_2^2 E(X^2(t_2))$$
$$= \mathrm{tr}\{\hat{\rho}(\alpha_1\hat{x}(t_1) + \alpha_2\hat{x}(t_2))^2\}$$
$$= \alpha_1^2\,\mathrm{tr}\{\hat{\rho}(\hat{x}(t_1))^2\} + \alpha_1\alpha_2$$
$$\times \mathrm{tr}\{\hat{\rho}(\hat{x}(t_1)\hat{x}(t_2) + \hat{x}(t_2)\hat{x}(t_1))\}$$
$$+ \alpha_2^2\,\mathrm{tr}\{\hat{\rho}(\hat{x}(t_2))^2\}. \tag{44}$$

The arbitrary character of α_1 and α_2 gives

$$E\{X(t_1)X(t_2)\} = \tfrac{1}{2}\,\mathrm{tr}\,[\hat{\rho}\{\hat{x}(t_1)\hat{x}(t_2) + \hat{x}(t_2)\hat{x}(t_1)\}]. \tag{45}$$

From (45), one obtains

$$(42) = \tfrac{1}{2}\lim_{s,\tau\to 0} \mathrm{tr}\left\{\hat{\rho}\left\{\left[\frac{\hat{x}(t+s)-\hat{x}(t)}{s}\right]\right.\right.$$
$$\times\left[\frac{\hat{x}(t'+\tau)-\hat{x}(t')}{\tau}\right]$$
$$\left.\left. + \left[\frac{\hat{x}(t'+\tau)-\hat{x}(t')}{\tau}\right]\left[\frac{x(t+s)-x(t)}{s}\right]\right\}\right\}. \tag{45'}$$

Under the stated conditions this limit exists and is

$$\tfrac{1}{2}\,\mathrm{tr}\,[\hat{\rho}\{\dot{\hat{x}}(t)\dot{\hat{x}}(t') + \dot{\hat{x}}(t')\dot{\hat{x}}(t)\}]. \tag{46}$$

One may ask whether an operator-valued real function $\hat{x}(t)$ can exist fulfilling all the required conditions. We have already mentioned that if $\hat{x}$ and $\hat{p}$ are the position and momentum operators in one dimension, respectively, and $\hat{x}(t) = h(t)\hat{x} + g(t)\hat{p} + \eta(t)I$, where $h(t)$, $g(t)$, and $\eta(t)$ are real functions, any real linear combination of the $\hat{x}(t)$ is e.s.a. on the Schwartz space $S(R)$.[14] Furthermore, if $h(t)$, $g(t)$, and $\eta(t)$ are derivable, $\dot{\hat{x}}(t) = \dot{h}(t)\hat{x} + \dot{g}(t)\hat{p} + \dot{\eta}(t)I$ and any real linear combination of the $\hat{x}(t)$ and the $\dot{\hat{x}}(t)$ is e.s.a. on $S(R)$. Moreover, the $\hat{x}(t)$ and the derivatives to all orders (if they existed) leave $S(R)$ invariant.

Remark: We know that the CWC in one dimension assigns to $\hat{\rho}$ a signed measure μ on the phase space R^2. Here R^2 can naturally be viewed as the Cartesian product of the ranges of the measurable functions representing, respectively, the position Q and the momentum P of a one-dimensional classical free particle. Here μ represents the quantum state of the particle given by $\hat{\rho}$ in the Hilbert space formalism. If μ were positive definite, the quantum mechanical state $\hat{\rho}$ would be equivalent to the classical statistical state given by μ on the phase space R^2. The CWC gives the following relation:

$$E\{e^{i(\alpha Q+\beta P)}\}=\int_{\Omega}e^{i(\alpha Q+\beta P)}d\mu$$
$$=\int_{\Omega}e^{i(\alpha q+\beta p)}\rho(q,p)dq\,dp$$
$$=\mathrm{tr}\{\hat{\rho}e^{i(\alpha\hat{x}+\beta\hat{p})}\}. \tag{47}$$

The density $\rho(q,p)$ is called the Wigner function[5] associated to the operator $\hat{\rho}$.

Assume now that $\hat{x}(t)=h(t)\hat{x}+g(t)\hat{p}+\eta(t)I$ and take $Y(t)=h(t)Q+g(t)P+\eta(t)\mathscr{I}$, where $\mathscr{I}$ maps R^2 into 1. Since we know $\rho(q,p)$, the joint distribution functions of the $Y(t)$ can be calculated, provided that μ were bounded. Let $X(t)$ be any stochastic process having the same distribution functions as $Y(t)$. The $X(t)$ and $\hat{x}(t)$ are related through a GWC.

The proof is based on the idea according to which the joint distribution functions fix the joint characteristic functions uniquely, if two stochastic processes have the same distribution functions, they have the same characteristic functions. Hence

$$\begin{aligned}&E\{\exp(i\{\alpha_1X(t_1)+\cdots+\alpha_nX(t_n)\})\}\\&\quad=E\{\exp(i\{\alpha_1[h(t_1)Q+g(t_1)P+\eta(t_1)\mathscr{I}]+\cdots\\&\qquad+\alpha_n[h(t_n)Q+g(t_n)P+\eta(t_n)\mathscr{I}]\})\}\\&\quad=\mathrm{tr}\{\hat{\rho}\exp(i\{\alpha_1[h(t_a)\hat{x}+g(t_1)\hat{p}+\eta(t_1)I]+\cdots\\&\qquad+\alpha_n[h(t_n)\hat{x}+g(t_n)\hat{p}+\eta(t_n)I]\})\}\\&\quad=\mathrm{tr}\{\hat{\rho}\exp(i\{\alpha_1\hat{x}(t_1)+\cdots+\alpha_n\hat{x}(t_n)\})\}.\end{aligned} \tag{48}$$

IV. QUADRATIC HAMILTONIANS AND VERITABLE PROCESSES

This section deals with a particular case. Here $\hat{x}(t)$ represents the position operator in the Heisenberg picture. The evolution from $\hat{x}(0)$ to $\hat{x}(t)$ is given by a time-independent Hamiltonian H. We assume that H is a quadratic function of the position and the momentum, i.e., $H=\alpha\hat{p}^2+\beta x^2+\delta(\hat{p}\hat{x}+\hat{q}\hat{x})+\gamma\hat{p}+\eta\hat{x}+\epsilon$. Here $\hat{\rho}$ is usually a positive trace class operator on $\mathscr{H}$, although its positivity is not necessarily required. The question we want to pose here is the following: If $\hat{x}(t)$ is related to a stochastic process $X(t)$ through the GWC, when is this process veritable? The answer obviously depends on $\hat{\rho}$.

If $X(t)$ were veritable, we could give a physical meaning to it whenever $\hat{\rho}$ is positive. For any $t\in J$, the distribution function of $X(t)$ would give the probability of finding a classical particle in some region of the configuration space. This classical particle has at any $t\in J$ the same expectation values for the position as a quantum particle evolving under the action of the Hamiltonian H and whose state in the Heisenberg picture is given by the positive trace class operator $\hat{\rho}$.

If $X(t)$ were not veritable or $\hat{\rho}$ were not positive, we could not give a physical meaning to $X(t)$.

The process $X(t)$ is veritable if and only if its joint density functions are positive definite. We shall calculate these joint densities for the case of a quadratic Hamiltonian. We start with the most simple cases including those of the free particle and the harmonic oscillator before solving the problem in its full generality. We finally find a sufficient condition for these density functions to be positive.

In the case of N dimensions, the position operator has N components $(\hat{x}_1(t),\ldots,\hat{x}_N(t))$ and the condition for the positivity of the joint densities is the same as in the one-dimensional case.

A. The one-dimensional case

1. Calculus of $\rho(x,t)$

In order to find the densities of the random variables in the process $X(t)$, we assume that $\hat{\rho}$ is positive first as in (2). Thus we have

$$\hat{\rho}=\sum_{k=1}^{\infty}\lambda_k|\psi_k\rangle\langle\psi_k|$$

with $\lambda_k\geqslant 0$, and (2) gives

$$E\{e^{i\alpha X(t)}\}=\int_{-\infty}^{\infty}e^{i\alpha x}\rho(x,t)dx=\mathrm{tr}\{\hat{\rho}e^{i\alpha x(t)}\}$$
$$=\sum_{k=1}^{\infty}\lambda_k\langle\psi_k|e^{i\alpha\hat{x}(t)}|\psi_k\rangle. \tag{49}$$

In the Schrödinger representation for states and observables, ψ_k is a function in $L^2(R)$ and $\hat{x}(0)$ is the multiplication by the variable x. Furthermore, if we use the Schrödinger picture, we have that

$$\langle\psi_k|e^{i\alpha\hat{x}(t)}|\psi_k\rangle=\int_{-\infty}^{\infty}|\psi_k(x,t)|^2e^{i\alpha x}\,dx. \tag{50}$$

Hence

$$\int_{-\infty}^{\infty}e^{i\alpha x}\rho(x,t)dx=\sum_{k=1}^{\infty}\lambda_k\int_{-\infty}^{\infty}|\psi_k(x,t)|^2e^{i\alpha x}\,dx. \tag{51}$$

Since $\lambda_k\geqslant 0$ and $\Sigma_{k=1}^{\infty}\lambda_k=1$, we can apply the monotonic convergence theorem so as to find the following result:

$$\int_{-\infty}^{\infty}e^{i\alpha x}\rho(x,t)dx=\int_{-\infty}^{\infty}\sum_{k=1}^{\infty}\lambda_k|\psi_k(x,t)|^2e^{i\alpha x}\,dx. \tag{52}$$

Hence

$$\rho(x,t)=\sum_{k=1}^{\infty}\lambda_k|\psi_k(x,t)|^2. \tag{53}$$

Note that this result is independent on the evolution Hamiltonian H. The case in which $\hat{\rho}$ is normal but not positive is not more involved and yields the same result. However, $\rho(x,t)$ is positive if $\hat{\rho}$ is positive, as is clear from (53).

2. Calculus of the joint densities for the free particle

In the present case the Hamiltonian is $H=\hat{p}^2/2m$ and the position and the momentum operators in the Heisenberg picture are

$$\hat{x}(t)=\hat{x}(0)+\hat{p}(0)(t/m),\quad \hat{p}(t)=\hat{p}(0). \tag{54}$$

To find the joint densities we make use of Eq. (6). Relations (54) give

$$\mathrm{tr}\{\hat\rho\exp(i\{\alpha_1\hat x(t_1)+\cdots+\alpha_n\hat x(t_n)\})\}$$
$$=\mathrm{tr}\{\hat\rho\exp(i\{(\alpha_1+\cdots+\alpha_n)\hat x+(1/m)(\alpha_1t_1+\cdots+\alpha_nt_n)\hat p\})\},\tag{55}$$

where $\hat x=\hat x(0)$ and $\hat p=\hat p(0)$ for simplicity. If we write

$$\alpha=\sum_{k=1}^n\alpha_k\quad\text{and}\quad\beta=\frac{1}{m}\sum_{k=1}^n\alpha_kt_k,\tag{56}$$

then

$$(55)=\mathrm{tr}\{\hat\rho\,e^{i\{\alpha\hat x+\beta\hat p\}}\}.\tag{57}$$

Therefore, (6) yields

$$\rho(x_1,t_1;\ldots;x_n,t_n)$$
$$=\frac{1}{(2\pi)^n}\int_{R^n}d\alpha_1,\ldots,d\alpha_n\times\exp(-i(\alpha_1x_1+\cdots+\alpha_nx_n))\mathrm{tr}\{\hat\rho e^{i(\alpha\hat x+\beta\hat p)}\},\tag{58}$$

where β contains the dependence on $t_1,\ldots,t_n$.

To perform the integration in (58), we have to change variables:

$$\alpha_1x_1+\cdots+\alpha_nx_n$$
$$=\alpha A+\beta B+\alpha_3C_3+\cdots+\alpha_nC_n$$
$$=\alpha_1A+\cdots+\alpha_nA+(\alpha_1t_1/m)B+\cdots+(\alpha_nt_n/m)B+\alpha_3C_3+\cdots+\alpha_nC_n.\tag{59}$$

Since $\alpha_1,\ldots,\alpha_n$ are arbitrary real numbers, we obtain the following equations:

$$\begin{aligned}&A+t_1B/m=x_1,\\&A+t_2B/m=x_2,\\&A+t_3B/m+C_3=x_3,\\&\quad\vdots\\&A+t_nB/m+C_n=x_n,\end{aligned}\tag{60}$$

from which we find the values of A, B, and C_k:

$$\begin{aligned}&A=x_1-t_1[(x_2-x_1)/(t_2-t_1)],\\&B=m[(x_2-x_1)/(t_2-t_1)],\\&C_k=x_k-x_1-(t_k-t_1)\times[(x_2-x_1)/(t_2-t_1)],\quad k\geqslant2.\end{aligned}\tag{61}$$

Here B is the mean value of the momentum of a classical free particle with mass m moving from x_1 to x_2 in a time interval t_2-t_1, and A and C_k represent positions of this particle.

We relabel the variables as follows:

$$\begin{aligned}&\alpha=\beta_1,\quad\beta=\beta_2,\quad\alpha_3=\beta_3,\quad\ldots,\quad\alpha_n=\beta_n;\\&A=S_1,\quad B=S_2,\quad C_3=S_3,\quad\ldots,\quad C_n=S_n.\end{aligned}\tag{62}$$

In order to write the integral in (58) in terms of these new variables, we first need to find the Jacobian corresponding to the change of variables (62). The inverse of this Jacobian is

$$\begin{vmatrix}1&1&1&\cdots&1\\t_1/m&t_2/m&t_3/m&\cdots&t_n/m\\0&0&1&&0\\\vdots&\vdots&\vdots&\vdots&\vdots\\0&0&0&&1\end{vmatrix}=(t_2-t_1)/m.\tag{63}$$

Hence

$$\rho(x_1,t_1,\ldots;x_n,t_n)=\frac{1}{(2\pi)^n}\frac{m}{|t_2-t_1|}\int_{R^n}d\beta_1,\ldots,d\beta_n\exp(-i(\beta_1S_1+\cdots+\beta_nS_n))\mathrm{tr}\{\hat\rho\exp(i(\beta_1\hat x+\beta_2\hat p))\}$$
$$=\frac{1}{(2\pi)^2}\frac{m}{|t_2-t_1|}\int_{R^2}d\beta_1\,d\beta_2\exp(-i(\beta_1S_1+B_2S_2))\mathrm{tr}\{\hat\rho\exp(i(\beta_1\hat x+\beta_2\hat p))\}$$
$$\times\frac{1}{2\pi}\int_{-\infty}^{\infty}d\beta_3\,e^{-i\beta_3S_3}\times\cdots\times\frac{1}{2\pi}\int_{-\infty}^{\infty}d\beta_n\,e^{-i\beta_nS_n}$$
$$=\frac{1}{(2\pi)^2}\frac{m}{|t_2-t_1|}W_{\hat\rho}(S_1,S_2,0)\prod_{k=3}^n\delta(S_k),\tag{64}$$

where

$$W_{\hat\rho}(S_1,S_2,0)=\int_{R^2}d\beta_1\,d\beta_2\exp(-i(\beta_1S_1+\beta_2S_2))\times\mathrm{tr}\{\hat\rho\exp(i(\beta_1\hat x+\beta_2\hat p))\}\tag{65}$$

is the Wigner function associated to the state $\hat\rho$.

From (64) and (65) we conclude that the process $X(t)$ is veritable if and only if the following propositions are fulfilled:

(1) the Wigner function for $\hat\rho$ is positive at $t=0$, and (2) the sum in (53) is positive.

This happens in particular if $\hat\rho$ is a Gaussian pure state.[15]

3. The case of the harmonic oscillator

Here $H=\hat p^2/2m+(mw^2/2)\hat x^2$ and

$$\begin{aligned}&\hat x(t)=\hat x(0)\cos wt+\hat p(0)(\sin wt)/mw,\\&\hat p(t)=-\hat x(0)mw\sin wt+\hat p(0)\cos wt.\end{aligned}\tag{66}$$

The procedures to find $\rho(x_1,t_1;\ldots;x_n,t_n)$ are always the same. After a more or less lengthy calculation, we find

$$\rho(x_1,t_1;\ldots;x_n,t_n)$$

$$= \frac{1}{(2\pi)^2} \frac{mw}{|\sin[w(t_2-t_1)]|} \prod_{k=3}^{n} \delta(S_k) W_{\hat{\rho}}(S_1,S_2,0), \tag{67}$$

which is well defined provided that $w(t_2-t_1) \neq \pi k$ with k integer and also that the S_k be well defined. We see again that a sufficient condition for $X(t)$ to be veritable is the positivity of the Wigner function associated to $\hat{\rho}$ at $t=0$. Here, the S_k have the following form:

$$S_1 = \frac{x_1}{\cos(wt_1)} \left\{ \frac{\tan(wt_2)}{\tan(wt_2)-\tan(wt_1)} \right\} - \frac{x_2}{\cos(wt_2)} \left\{ \frac{\tan(wt_1)}{\tan(wt_2)-\tan(wt_1)} \right\},$$

$$S_2 = \frac{mw}{\tan(wt_2)-\tan(wt_1)} \left\{ \frac{x_2}{\cos(wt_2)} - \frac{x_1}{\cos(wt_1)} \right\},$$

$$S_k = x_k + x_1 \left\{ \frac{\sin(wt_k)}{\cos(wt_1)} - \frac{\cos(wt_k)}{\cos(wt_1)} \tan(wt_2) \right\} \times \frac{1}{\tan(wt_2)-\tan(wt_1)}$$

$$+ x_2 \left\{ \frac{\cos(wt_k)}{\cos(wt_2)} \tan(wt_1) - \frac{\sin(wt_k)}{\cos(wt_2)} \right\} \times \frac{1}{\tan(wt_2)-\tan(wt_2)}, \quad k \geqslant 2. \tag{68}$$

If the Hamiltonian was of the form $H=\hat{p}^2-\hat{x}^2$ or $H=\hat{p}^2+\alpha\hat{x}$, we would obtain a similar result. Thus we could conjecture that if H were any quadratic Hamiltonian we would arrive at the same conclusion. This conjecture is true and we shall prove it in the following two subsections.

4. The general quadratic Hamiltonian in one dimension

Assume that $H = \alpha\hat{p}^2 + \beta\hat{x}^2 + \gamma(\hat{x}\hat{p}+\hat{p}\hat{x}) + \delta\hat{x} + \eta\hat{p} + \epsilon$. This Hamiltonian gives us a simple behavior for $\hat{x}(t)$. After having solved the equations of motion, we obtain

$$\hat{x}(t) = f(t)\hat{x}(0) + g(t)\hat{p}(0) + h(t)I, \tag{69}$$

where $f(t)$, $g(t)$, and $h(t)$ are real functions on t, and I is the identity on $\mathscr{H}$.

In this situation we arrive at

$$\rho(x_1t_1;\ldots;x_n,t_n) = \frac{1}{(2\pi)^2} \frac{1}{|g(t_2)f(t_1)-g(t_1)f(t_2)|} \prod_{k=3}^{n} \delta(S_k) W_{\hat{\rho}}(S_1,S_2,0), \tag{70}$$

where

$$S_1 = \frac{[x_2-h(t_2)]g(t_1) - [x_1-h(t_1)]g(t_2)}{g(t_1)f(t_2)-g(t_2)f(t_1)},$$

$$S_2 = \frac{[x_1-h(t_1)]f(t_2) - [x_2-h(t_2)]f(t_1)}{g(t_1)f(t_2)-g(t_2)f(t_1)}, \tag{71}$$

$$S_k = x_k - h(t_k) - f(t_k) \left\{ \frac{[x_2-h(t_2)]g(t_1) - [x_1-h(t_1)]g(t_2)}{g(t_1)f(t_2)-g(t_2)f(t_1)} \right\} - g(t_k) \left\{ \frac{[x_1-h(t_1)]f(t_2) - [x_2-h(t_2)]f(t_1)}{g(t_1)f(t_2)-g(t_2)f(t_1)} \right\}.$$

Equation (70) leads to the same conclusion: if $\hat{\rho}$ is positive and $g(t_2)f(t_1) \neq g(t_1)f(t_2)$, the finite-dimensional distribution functions are positive if and only if the Wigner function for $\hat{\rho}$ is positive at $t=0$ ($n \geqslant 2$).

B. The N-dimensional case

Here we want to obtain the density given by formula (10). First, we have to find a new expression for the trace,

$$\mathrm{tr}\{\hat{\rho}\exp\{i(\alpha_{11}\hat{x}_1(t_1) + \cdots + \alpha_{Ns}\hat{x}_N(t_s))\}\}, \tag{72}$$

for which we need to write $\hat{x}_k(t)$ as a function of the coordinates of the position $(\hat{x}_1(0),\ldots,\hat{x}_n(0))$ and the momentum $(\hat{p}_1(0),\ldots,\hat{p}_n(0))$ at $t=0$.

The transition from $\hat{x}(0)$ to $\hat{x}(t)$ is due to a dynamics given by a quadratic Hamiltonian which is $H = \mu^t B\mu + C^t\mu + D$, where

$$\mu = \begin{pmatrix} \hat{x}_1(t) \\ \vdots \\ \hat{x}_N(t) \\ \hat{p}_1(t) \\ \vdots \\ \hat{p}_N(t) \end{pmatrix}.$$

Here B is a symmetric $2N \times 2N$ real matrix, C is a $2N \times 1$ real matrix, and D is a real function. The equations of the motion are ($\hbar = 1$)

$$i\dot{\hat{x}}_k(t) = [\hat{x}_k(t),H], \quad i\dot{\hat{p}}_k(t) = [p_k(t),H]. \tag{73}$$

Equations (73) yield the following linear system:

$$\begin{pmatrix} \dot{\hat{x}}_1(t) \\ \vdots \\ \dot{\hat{x}}_N(t) \\ \dot{\hat{p}}_1(t) \\ \vdots \\ \dot{\hat{p}}_N(t) \end{pmatrix} = M \begin{pmatrix} \hat{x}_1(t) \\ \vdots \\ \hat{x}_N(t) \\ \hat{p}_1(t) \\ \vdots \\ \hat{p}_N(t) \end{pmatrix} + T. \tag{74}$$

Here M is a $2N \times 2N$ real matrix and T is a $2N \times 1$ real matrix. The system in (74) can be easily integrated. Its solutions are of the form

$$\hat{x}_i(t) = \sum_{k=1}^{N} \{f_{ik}(t)\hat{x}_k(0) + g_{ik}(t)\hat{p}_k(0)\} + h_i(t)I \tag{75}$$

and (72) becomes

$$\mathrm{tr}\{\hat{\rho}\exp(i\{\gamma_1\hat{x}_1(0) + \cdots + \gamma_N\hat{x}_N(0) + \delta_1\hat{p}_1(0) + \cdots + \delta_N\hat{p}_N(0) + \xi I\})\}, \tag{76}$$

where $\gamma_1,\ldots,\gamma_N$, $\delta_1,\ldots,\delta_N$, depend on $t_1,\ldots,t_s$ and $\alpha_{11},\ldots,\alpha_{Ns}$. This dependence is given by a suitable change of variables transforming (10) into the following formula for the joint densities:

$$\begin{aligned}
&\rho(x_{11},\ldots,x_{N1},t_1;\ldots;x_{1s},\ldots,x_{Ns},t_s) \\
&\quad = \frac{|J|}{(2\pi)^{N\times s}} \int dr_1\cdots dr_{Ns}\exp(-i(r_1q_1 + \cdots + r_{Ns}q_{Ns})) \\
&\qquad \times \mathrm{tr}\{\hat{\rho}\exp(i\{r_1\hat{x}_1(0) + \cdots + r_N\hat{x}_N(0) + r_{N+1}\hat{p}_1(0) + \cdots + r_{2N}\hat{p}_N(0) + r_{2N+1}I\})\} \\
&\quad = \frac{|J|}{(2\pi)^{2N}}\delta(1 - q_{2N+1}) \sum_{k=2N+2}^{N\times s} \delta(q_k)\, W_{\hat{\rho}}(q_1,q_{N+1};\ldots;q_N,q_{N+N};0), \\
&\qquad r_i = \gamma_i, \quad i = 1,\ldots,N, \quad r_k = \delta_{k-N}, \quad k = N+1,\ldots,2N, \quad r_{2N+1} = \xi,
\end{aligned} \tag{77}$$

where

$$\begin{aligned}
&W_{\hat{\rho}}(q_1,q_{N+1};\ldots;q_N,q_{N+N};0) \\
&\quad = \int d\gamma_1,\ldots,d\gamma_N d\delta_1,\ldots,d\delta_N \\
&\qquad \times \exp(-i(\gamma_1q_1 + \cdots + \delta_Nq_{2N})) \\
&\qquad \times \mathrm{tr}\{\hat{\rho}\exp(i\{\gamma_1\hat{x}_1(0) + \cdots + \delta_N\hat{p}_N(0)\})\}
\end{aligned} \tag{78}$$

is the N-dimensional Wigner function at $t = 0$. Here $|J|$ is the Jacobian of the change of the variables. It depends on $t_1,\ldots,t_s$ and on the Hamiltonian H as well as the q_k.

A detailed calculation of the q_k is not necessary to conclude that, after (77), the joint densities are positive if and only if the N-dimensional Wigner function is positive at $t = 0$.

C. Joint densities in phase space

Assume that the stochastic vector $(X(t),P(t))$ and $(\hat{x}(t),\hat{p}(t))$ are related through a GWC, where $\hat{x}(t)$ and $\hat{p}(t)$ are again the position and momentum, respectively, of a quantum Hamiltonian. The stochastic vector $(X(t),P(t))$ is veritable if and only if the joint densities $\rho(x_1,p_1,t_1;\ldots;x_m,p_m,t_m)$ are positive. Performing the same kind of calculations, we find out that the positive of the densities is equivalent to the positivity of the corresponding Wigner function at $t = 0$. This result is immediately extended to the N-dimensional case.

V. TIME-INDEPENDENT HAMILTONIANS IN ONE DIMENSION

So far, we have studied the case in which H is a quadratic Hamiltonian. The objective of the present section is the study of the situation produced by a general time-independent Hamiltonian in one dimension and of the form $H = p^2/2m + V(x)$. Quantum mechanics gives us the time development for the observable position as

$$\hat{x}(t) = e^{iHt}\hat{x}(0)e^{-iHt}. \tag{79}$$

Assume that $\hat{x}(0)$ and H have a common dense domain $\mathscr{D}$ stable under the action of these operators. From (79) we conclude that $\hat{x}(t)$ is strongly differentiable as a function of t and the following equations make sense on $\mathscr{D}$:

$$\begin{aligned}
&i\dot{\hat{x}}(t) = [\hat{x}(t),H], \\
&\hat{x}(t + \Delta t) = x(t) - i[\hat{x}(t),H]\Delta t + O(\Delta t).
\end{aligned} \tag{80}$$

Since $[\hat{x}(t),H] = i\hat{p}(t)/m$, (80) yields

$$\hat{x}(t + \Delta t) = \hat{x}(t) + (\Delta t/m)\hat{p}(t) + O(\Delta t). \tag{81}$$

Now, we are seeking a necessary condition for $X(t)$ to be veritable. Equation (6) gives us the following equation:

$$\begin{aligned}
&\rho(x,t;x',t + \Delta t) \\
&\quad = \frac{1}{(2\pi)^2}\int d\alpha_1\, d\alpha_2 \exp(-i(\alpha_1x + \alpha_2x')) \\
&\qquad \times \mathrm{tr}\{\hat{\rho}\exp(i\{\alpha_1\hat{x}(t) + \alpha_2\hat{x}(t + \Delta t)\})\} \\
&\quad = \frac{1}{(2\pi)^2}\int d\alpha_1\, d\alpha_2 \exp(-i(\alpha_1x + \alpha_2x')) \\
&\qquad \times \mathrm{tr}\{\hat{\rho}\exp(i\{(\alpha_1 + \alpha_2)\hat{x}(t) \\
&\qquad + (\alpha_2\Delta t/m)\hat{p}(t) + O(\Delta t)\})\},
\end{aligned} \tag{82}$$

where we have made use of (81). Now, we perform the change of variables

$$\alpha = \alpha_1 + \alpha_2, \quad \beta = \alpha_2(\Delta t/m), \tag{83}$$

whose Jacobian is $\Delta t/m$. Thus

$$\rho(x,t;x',t+\Delta t)$$
$$=\frac{1}{(2\pi)^2}\frac{m}{|\Delta t|}\int d\alpha\, d\beta \times\exp(-i\{\alpha x+\beta[(m/\Delta t)(x'-x)]\}) \times\mathrm{tr}\{\hat\rho\exp(i\{\alpha\hat x(t)+\beta\hat p(t)+O(\Delta t)\})\}. \quad (84)$$

From a physical point of view, if $X(t)$ is veritable, $\rho(x,t;x',t+\Delta t)$ is the joint probability density of finding the corresponding classical particle at x at the time t and x' at the time $t+\Delta t$. Therefore, the joint density $\rho(x,t;x',t)$ does not have physical meaning when $x\neq x'$. In addition, if $\Delta t\to 0$ the point x' has to approach x, if we want to be consistent with this physical interpretation. Thus $p(\Delta t)=m(x'-x)/\Delta t$ goes to the classical momentum of the particle at x when $\Delta t\to 0$.

Obviously, if $\rho(x,t;x',t+\Delta t)$ has to be positive for any values of t, Δt, x, and x', it has also to be positive at the limit when $\Delta t\to 0$. Hence

$$0\leqslant\lim_{\Delta t\to 0}\int d\alpha\, d\beta\exp(-i\{\alpha x+\beta m/\Delta t(x'-x)\}) \times\mathrm{tr}\{\hat\rho\exp(i\{\alpha\hat x(t)+\beta\hat p(t)+O(\Delta t)\})\}$$
$$=\int d\alpha\, d\beta\exp(-i\{\alpha x+\beta p\}) \times\mathrm{tr}\{\hat\rho\exp(i\{\alpha\hat x(t)+\beta\hat p(t)\})\}$$
$$=W_{\hat\rho}(x,p,t). \quad (85)$$

Thus a necessary condition for $X(t)$ to be veritable is that the Wigner function for $\hat\rho$ be positive at any value of the time.

When $\hat\rho$ is a pure state, Soto and Claverie[16] have proved the following statement: The positivity of the Wigner function at $t=0$ guarantees its positivity at any $t>0$ if H is a quadratic Hamiltonian of the type $\alpha p^2+\beta q^2+\gamma q+\delta$. Conversely, if H is not of this kind, the two-dimensional joint functions are not positive definite for any value of time, and, therefore, $X(t)$ cannot be veritable, if $\hat\rho$ is a pure state.

To close this section, we give here a new characterization of the Wigner function. Consider the following function:

$$F(x,p,t)=\lim_{\Delta t\to 0^+}\int_{-\infty}^{x}dx' \times\int_{-\infty}^{x'+p\Delta t/m}dx''\,\rho(x',t;x'',t+\Delta t)$$
$$=\lim_{\Delta t\to 0^+}F_{\Delta t}(x,p,t). \quad (86)$$

Under sufficient regularity conditions, we can take on $F_{\Delta t}(x,p,t)$ partial derivatives with respect to the variables x and p, so as to have

$$\frac{\partial^2 F_{\Delta t}(x,p,t)}{\partial x\,\partial p}=\frac{\Delta t}{m}\rho\left(x,t;x+p\frac{\Delta t}{m},t+\Delta t\right)$$
$$=\frac{1}{(2\pi)^2}\frac{\Delta t}{|\Delta t|}\int d\alpha\, d\beta\, e^{-i\{\alpha x+\beta p\}} \times\mathrm{tr}\{\hat\rho\exp(i\{\alpha\hat x(t)+\beta\hat p(t)+O(\Delta t)\})\}. \quad (87)$$

Therefore

$$\lim_{\Delta t\to 0^+}\frac{\partial F_{\Delta t}(x,p,t)}{\partial x\,\partial p}=\frac{1}{(2\pi)^2}W_{\hat\rho}(x,p,t). \quad (88)$$

Note that, if the two-dimensional joint densities are positive, the Wigner function is also positive.

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APPENDIX A: PROOF OF LEMMA II

Let us give the proof for $n=1$. For higher values of n, this proof does not involve new arguments. Thus assume that

$$\mathrm{tr}\{\hat\rho|A|\}<\infty. \quad (A1)$$

Since A is self-adjoint, the spectral theorem gives a positive measure μ_k for each $\psi_k\in\mathscr{D}(A)$ such that

$$\langle\psi_k|A\psi_k\rangle=\int_{-\infty}^{\infty}\lambda\,d\mu_k \quad (A2)$$

and

$$\langle\psi_k||A|\psi_k\rangle=\int_{-\infty}^{\infty}|\lambda|\,d\mu_k. \quad (A3)$$

Let

$$\hat\rho=\sum_{k=1}^{\infty}\lambda_k|\psi_k\rangle\langle\psi_k|$$

with $\psi_k\in\mathscr{D}(A)$ and assume first that $\hat\rho$ is positive. Then, we have

$$\mathrm{tr}\{\hat\rho|A|\}=\sum_{k=1}^{\infty}\lambda_k\int_{-\infty}^{\infty}|\lambda|\,d\mu_k. \quad (A4)$$

Since $\Sigma_{k=1}^{\infty}\lambda_k<\infty$, the Lebesgue theorem gives

$$(A4)=\int_{-\infty}^{\infty}|\lambda|\sum_{k=1}^{\infty}\lambda_k\,d\mu_k=\int_{-\infty}^{\infty}|\lambda|\,d\mu, \quad (A5)$$

where $d\mu=\Sigma_{k=1}^{\infty}\lambda_k\,d\mu_k$ is a finite measure on R. Now take

$$\mathrm{tr}\{\hat\rho e^{i\alpha A}\}=\sum_{k=1}^{\infty}\lambda_k\langle\psi_k|e^{i\alpha A}\psi_k\rangle$$
$$=\sum_{k=1}^{\infty}\lambda_k\int_{-\infty}^{\infty}e^{i\alpha\lambda}\,d\mu_k=\int_{-\infty}^{\infty}e^{i\alpha\lambda}\,d\mu. \quad (A6)$$

Our next goal is to obtain the derivative of (A6) with respect to α at zero. This derivative can be introduced inside the last integral in (A6) if

$$(1)\quad\int_{-\infty}^{\infty}|i\lambda|\,|e^{i\alpha\lambda}|\,d\mu<\infty, \quad (A7)$$

$$(2)\quad\left|\frac{\partial}{\partial\alpha}e^{i\alpha\lambda}\right|\leqslant f(\lambda)\in L^1(d\mu). \quad (A8)$$

Here (1) and (2) are fulfilled, since $f(\lambda)=\lambda$ and $\int_{-\infty}^{\infty}|\lambda|\,d\mu<\infty$. Thus

$$\frac{d}{d\alpha}\operatorname{tr}\hat{\rho}e^{i\alpha A}\Big|_{\alpha=0}$$
$$=\frac{d}{d\alpha}\int_{-\infty}^{\infty}e^{i\alpha\lambda}d\mu\Big|_{\alpha=0}$$
$$=\int_{-\infty}^{\infty}i\lambda\,d\mu=i\sum_{k=1}^{\infty}\lambda_k\int_{-\infty}^{\infty}d\mu_k=i\operatorname{tr}\{\hat{\rho}A\}. \tag{A9}$$

If $\hat{\rho}$ were any normal trace class operator, the procedures of the demonstration would be identical. The only peculiarity to be noted in such a case is that μ would then be a complex bounded measure.

APPENDIX B: PROOF OF LEMMA III

Assume that $\hat{\rho}$ is positive. Then,

$$\operatorname{tr}\{\hat{\rho}A^2\}=\sum_{k=1}^{\infty}\lambda_k\langle\psi_k|A^2\psi_k\rangle=\sum_{k=1}^{\infty}\lambda_k\|A\lambda_k\|^2, \tag{B1}$$

$$\operatorname{tr}\{\hat{\rho}B^2\}=\sum_{k=1}^{\infty}\lambda_k\|B\psi_k\|^2, \tag{B2}$$

$$\operatorname{tr}\{\hat{\rho}AB\}=\sum_{k=1}^{\infty}\lambda_k\langle\psi_k|AB\psi_k\rangle=\sum_{k=1}^{\infty}\lambda_k\langle A\psi_k|B\psi_k\rangle, \tag{B3}$$

$$|\operatorname{tr}\{\hat{\rho}AB\}|\leqslant\sum_{k=1}^{\infty}\lambda_k\|A\psi_k\|\,\|B\psi_k\|. \tag{B4}$$

We want to find a upper bound for the rhs in (B4). This can be easily done by noting that if a and b are positive numbers, we have

$$0\leqslant ab\leqslant\tfrac{1}{2}(a^2+b^2). \tag{B5}$$

Thus,

$$0\leqslant\sum_{k=1}^{\infty}\lambda_k\|A\psi_k\|\,\|B\psi_k\|$$
$$\leqslant\frac{1}{2}\left\{\sum_{k=1}^{\infty}\lambda_k(\|A\psi_k\|^2+\|B\psi_k\|^2)\right\}$$
$$=\frac{1}{2}\left\{\sum_{k=1}^{\infty}\lambda_k\|A\psi_k\|^2+\sum_{k=1}^{\infty}\lambda_k\|B\psi_k\|^2\right\}. \tag{B6}$$

If $\hat{\rho}$ were not positive, we would have to assume that

$$\sum_{k=1}^{\infty}|\lambda_k|\,\|A\psi_k\|^2$$

and

$$\sum_{k=1}^{\infty}|\lambda_k|\,\|B\psi_k\|^2$$

are both finite.

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$$\Delta=\{w\in\Omega/[X(t)](w)=[X(t_0)](w)\ \forall t\in J\}$$

is a closed set in Ω. Therefore if we consider in Ω its Borel σ algebra β, Δ is a measurable set. On (Ω,β) we can give a probability measure such that $P(\Delta)=1$. The process $X(t)$ fulfills the required condition.
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Effective potential determining one-dimensional Slater sum in independent-particle theory

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Hilton, March, and Curtis [Proc. R. Soc. London Ser. A **300**, 391 (1967)] have earlier focused on the utility of the effective potential $U(\mathbf{r},\beta)$ in determining the Slater sum $Z(\mathbf{r},\beta) = Z_0(\beta)\exp(-\beta U(\mathbf{r},\beta))$. Here an explicit, though highly nonlinear, partial differential equation is derived for determining the effective potential $U(x,\beta)$ in one-dimensional problems. Direct solution of this equation by power series expansion in β leads readily to Husimi's results obtained from off-diagonal density matrix calculations. Perturbation theory in the potential is also developed, and thereby it is shown that an infinite subseries of the Husimi expansion is readily summed, and that a scaling property is exhibited.

I. INTRODUCTION

This work is concerned with some formally exact results for the effective potential[1] $U(x,\beta)$ which determines the one-dimensional Slater sum

$$Z(x,\beta) = Z_0(\beta)\exp(-\beta U(x,\beta)). \tag{1}$$

In terms of the eigenfunctions $\psi_i(x)$ and the corresponding eigenvalues ϵ_i of the one-particle Hamiltonian

$$H = -(\hbar^2/2m)\nabla^2 + V(x), \tag{2}$$

the Slater sum is defined by

$$Z(x,\beta) = \sum_i \psi_i^*(x)\psi_i(x)\exp(-\beta\epsilon_i), \quad \beta = (k_B T)^{-1}, \tag{3}$$

$Z_0(\beta)$ in Eq. (1) being its free-particle value corresponding to $V(x) = 0$.

As was proved by March and Murray[2] in their treatment of central field problems, which, of course, corresponds to dealing with one-dimensional Schrödinger equations, the Bloch equation satisfied by the off-diagonal density matrix $C(x,x_0,\beta)$, defined by replacing $\psi_i(x)$ in Eq. (3) by $\psi_i(x_0)$,

$$HC = -\frac{\partial C}{\partial \beta}, \tag{4}$$

can be expanded about its diagonal $x_0 = x$ to yield the following partial differential equation for the Slater sum $Z(x,\beta)$:

$$\frac{\hbar^2}{8m} Z''' - \frac{\partial Z'}{\partial \beta} - VZ' - \frac{1}{2} V'Z = 0. \tag{5}$$

Though Eq. (5) is linear in Z, it has so far only proved possible to solve it for specific potentials $V(x)$, e.g., the harmonic oscillator with $V(x) = \frac{1}{2} m\omega^2 x^2$ in closed form. Since, for many purposes, one must have recourse to approximate methods, Ref. 1 will be followed here in seeking to determine $U(x,\beta)$. While in Ref. 1, and also in earlier work by Husimi,[3] $U(x,\beta)$ was calculated by expansions either in V or in β, but employing off-diagonal knowledge of $C(x,x_0,\beta)$, current interests in density functional theory prompt the investigation reported below of $U(x,\beta)$ from a purely diagonal approach.

II. DIAGONAL DIFFERENTIAL EQUATION FOR THE EFFECTIVE POTENTIAL

Returning to Eq. (1), and noting that the free-particle Slater sum $Z_0(\beta)$ can be found by inserting free-particle waves $\exp(ikx)$ and energies $\hbar^2 k^2/2m$ into Eq. (3) to yield

$$Z_0(\beta) = (m/2\pi\hbar^2\beta)^{1/2}, \tag{6}$$

one can insert Eqs. (1) and (6) into Eq. (5) to obtain the defining equation for $U(x,\beta)$ itself as

$$\begin{aligned}\frac{\hbar^2}{8m}\beta U''' - \beta\frac{\partial U'}{\partial\beta} + \frac{1}{2}V' - \frac{1}{2}U' &= \beta U'(V-U) - \beta^2 U'\frac{\partial U}{\partial\beta} \\ &\quad + \frac{3\hbar^2}{8m}\beta^2 U'U'' - \frac{\hbar^2}{8m}\beta^3 U'^3.\end{aligned} \tag{7}$$

This purely diagonal equation for the effective potential $U(x,\beta)$ can be viewed as the diagonal counterpart of the off-diagonal equation derived by Husimi[3] from the Bloch equation (4), and solved by him via a power series expansion in β.

III. APPROXIMATE SERIES SOLUTIONS OF THE DIAGONAL EQUATION FOR $U(x,\beta)$

Notwithstanding the highly nonlinear character of Eq. (7), let us first demonstrate, in establishing its usefulness, that all of Husimi's results are readily regained from it.

Writing

$$U(x,\beta) = u_0(x) + \beta u_1(x) + \beta^2 u_2(x) + \cdots, \tag{8}$$

one finds immediately from the $O(1)$ terms in Eq. (7) that

$$u_0'(x) = V'(x), \tag{9}$$

showing that the Thomas–Fermi approximation $U(x,\beta) \simeq V(x)$ is regained in this lowest-order treatment.

Proceeding to terms of $O(\beta)$, one finds similarly

$$(\hbar^2/8m)V''' - \tfrac{3}{2}u_1' = 0, \tag{10}$$

which reproduces immediately Husimi's first-order result

$$u_1(x) = (\hbar^2/12m)V''(x). \tag{11}$$

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Continuing to $O(\beta^2)$ one has

$$(\hbar^2/8m)u_1''' - \tfrac{5}{2}u_2' = -2V'u_1 + (3\hbar^2/8m)V'V'' \quad (12)$$

with solution, using Eq. (11) for u_1, which is readily verified to be

$$u_2 = \tfrac{1}{240}(\hbar^2/m)^2 V^{iv}(x) - (\hbar^2/24m)\{V'(x)\}^2. \quad (13)$$

The next useful step is to note that the leading terms in u_0, u_1, and u_2, etc., are all first order in the potential V. These are readily summed to all orders in β by returning to the diagonal equation (7) and noting that the right-hand side is of second and higher order in $V(x)$. Hence denoting the solution to first order in V by $U_1(x,\beta)$ one needs to solve

$$\frac{\hbar^2}{8m}\beta U_1'' - \beta\frac{\partial U_1}{\partial\beta} + \frac{1}{2}V - \frac{1}{2}U_1 = 0, \quad (14)$$

after inserting appropriate physical boundary conditions. Taking the Fourier transform with respect to x, to yield $\tilde{U}_1(p,\beta)$, one finds for potentials $V(x)$, which have a Fourier transform $\tilde{V}(p)$,

$$-\frac{\hbar^2p^2\beta}{8m}\tilde{U}_1 - \beta\frac{\partial\tilde{U}_1}{\partial\beta} + \frac{1}{2}\tilde{V} - \frac{1}{2}\tilde{U}_1 = 0. \quad (15)$$

Writing

$$\tilde{U}_1(p,\beta) = \tilde{V}(p)\tilde{f}(p,\beta) \quad (16)$$

yields

$$\frac{\partial\tilde{f}}{\partial\beta} + \left[\frac{1}{2\beta} + \frac{\hbar^2p^2}{8m}\right]\tilde{f} = \frac{1}{2\beta}. \quad (17)$$

Employing the integrating factor $\beta^{1/2}\exp\{(\hbar^2p^2/8m)\beta\}$, one finds the explicit form of $\tilde{f}(p,\beta)$ to be

$$\tilde{f}(p,\beta) = \beta^{-1/2}\exp\left(\frac{-\hbar^2p^2\beta}{8m}\right)\int^{\beta}\frac{1}{2}\beta^{1/2} \times\exp\left(\frac{\hbar^2p^2\beta}{8m}\right)d\beta. \quad (18)$$

In coordinate space, the product form (16) evidently corresponds to a convolution,[1]

$$U_1(x,\beta) = \int_{-\infty}^{\infty} V(x_1)f(x_1 - x,\beta)dx_1, \quad (19)$$

where $f(x_1 - x,\beta)$ can be found from Eq. (18) as

$$f(x_1 - x,\beta) = [1/2\beta Z_0(\beta)]\,\mathrm{erfc}\{\sqrt{2}|x_1 - x|/\sqrt{\beta}\}, \quad (20)$$

which, it is to be emphasized, has been derived by purely diagonal arguments. This result (19), with f given by (20), sums up the Husimi series in β to infinite order, to first order in V.

Evidently, returning to Eq. (7), one can determine the "correction" U_2 of $O(V^2)$ to U_1 in Eq. (19). The appropriate differential equation is

$$\frac{\hbar^2}{8m}\beta U_2''' - \beta\frac{\partial U_2'}{\partial\beta} - \frac{1}{2}U_2' = \beta U_1'(V - U_1) - \beta^2 U_1'\frac{\partial U_1}{\partial\beta} + \frac{3\hbar^2}{8m}\beta^2 U_1'U_1''. \quad (21)$$

This can, in fact, be solved, but the detail proliferates. The only case, so far, in which a closed solution to Eq. (7) has been achieved is for the harmonic oscillator example referred to above. Here it is readily verified that the form

$$Z(x,\beta) = \left(\frac{m}{2\pi\hbar^2\beta}\right)^{1/2}\left(\frac{\beta\hbar\omega}{\sinh(\beta\hbar\omega)}\right)^{1/2} \times\exp\left(-x^2\frac{m\omega}{\hbar}\tanh\left(\frac{1}{2}\beta\hbar\omega\right)\right), \quad (22)$$

derived by Uhlenbeck and Gropper[4] by directly performing the sum (3) using the known wave functions and energy levels corresponds to

$$U(x,\beta) = \frac{m\omega^2x^2}{\hbar\omega\beta}\tanh\left(\frac{1}{2}\hbar\omega\beta\right) - \frac{1}{2\beta}\ln\left(\frac{\hbar\omega\beta}{\sinh(\hbar\omega\beta)}\right) \quad (23)$$

and that this is an exact solution of Eq. (7) to all orders in V.

To summarize, Eq. (7) is the main result of the present work: it establishes a diagonal method for generalizing the Thomas–Fermi approximation $U(x,\beta) \simeq V(x)$, which is thereby demonstrated to be true in the limits of (a) sufficiently small β from Eqs. (8) and (9) for sufficiently slow spatial variations in $V(x)$ from Eq. (7). In the latter connection, it is worth emphasizing that Eq. (13), with f given by Eq. (14), shows that in the expression for U_1, the combination $V^{(2n)}(x)\beta^n$ always appears, with $V^{(n)}$ representing the nth derivative of $V(x)$. Presumably, similar scaling will be derivable in each order of the perturbation series and this may point to further progress in solving the nonlinear equation (7) for the effective potential.

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Electron density and Slater sum of a semi-infinite electron gas in d dimensions

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By taking the electron densities of semi-infinite electron gases in one and in three dimensions, and forming the Slater sum by the Laplace transform, it is shown that the Slater sum is the classical partition function in d dimensions, times a function independent of dimensionality. The electron density is thereby calculated for general dimensionality, as is the kinetic energy density. As a by-product, the dimensionality dependence of Friedel oscillations emerges in general form.

I. INTRODUCTION

There is currently considerable interest in describing many-electron systems by their electron density ρ. It seemed, therefore, to be of interest to study the inhomogeneous semi-infinite electron gases as a functional of dimensionality.

To introduce the study, consider the simplest wave mechanical problem: electrons moving freely within a one-dimensional box of length l, in the region $0<z<l$. Then with N electrons singly filling the lowest levels, the electron density is evidently

$$\rho_1(z)=\left(\frac{2}{l}\right)\sum_1^N \sin^2\frac{n\pi z}{l}. \tag{1}$$

One can calculate the sum exactly, and then pass to the semi-infinite electron gas limit $l\to\infty$, $N\to\infty$, $N/l\to\rho_{10}$, the bulk electron gas number of electrons per unit length. Or one can replace the summation over levels by an integration, and writing the highest (or Fermi) energy E as $k^2/2$ one finds readily

$$\rho_1(z)=\rho_{10}[1-[\sin(2kz)]/(2kz)]$$
$$=\rho_{10}[1-j_0(2kz)],\quad \rho_{10}=k/\pi, \tag{2}$$

where $j_l(x)$ denotes the l th-order spherical Bessel function.

As utilized extensively by March and Murray,[1] one can construct the Slater sum, which weights the square of the wave functions in Eq. (1) with the Boltzmann factor $\exp(-\beta\epsilon_n)$, by using the Laplace transform relation

$$Z(z,\beta)=\beta\int_0^\infty \rho(z,E)\exp(-\beta E)dE. \tag{3}$$

Inserting Eq. (2), and using the properties of Laplace transforms set out below, one finds

$$Z_1(z,\beta)=(2\pi\beta)^{-1/2}(1-\exp(-2z^2/\beta)). \tag{4}$$

Next, let us turn to the three-dimensional case, in which electrons are confined to the semi-infinite space $0<z<\infty$ by an infinite barrier in the (x,y) plane. This model was studied by Bardeen,[2] as a description of the electron distribution at a planar metal surface. His result for the electron density, written for comparison with Eq. (2) in terms of singly filled levels, is

$$\rho_3(z)=\rho_{30}(1-3j_1(2kz)/2kz),\quad \rho_{30}=k^3/6\pi^2. \tag{5}$$

Brown *et al.*[3] pointed out that, for this problem, the canonical density matrix could be derived by solving the Bloch equation and on the diagonal they obtained[3,4]

$$Z_3(z,\beta)=(2\pi\beta)^{-1}Z_1(z,\beta). \tag{6}$$

In fact, by taking the Bloch equation in d dimensions, it is readily shown that

$$Z_d(z,\beta)=(2\pi\beta)^{(1-d)/2}Z_1(z,\beta), \tag{7}$$

confirming that one can write for the d-dimensional case a factor related to the free-particle partition function per unit volume times a factor independent of dimensionality.

Starting from the form (7), one can now invert the Laplace transform relation (3), using the following identities:

$$\mathscr{L}^{-1}(\beta^{-n-1/2})=\frac{\pi^{-1/2}}{\frac{1}{2}\cdot\frac{3}{2}\cdots(n-\frac{1}{2})}\left(\frac{k^2}{2}\right)^{n-1/2} \tag{8}$$

and

$$\mathscr{L}^{-1}\frac{\exp(-2z^2/\beta)}{\beta^{(l+3/2)}}=\frac{(2\pi)^{3/2}}{2\pi^2}k^{2l+1}\frac{j_l(2kz)}{(2kz)^l}. \tag{9}$$

One needs to find

$$\rho_d(z)=[1/(2\pi)^{(d-1)/2}]\,\mathscr{L}^{-1}[1/\beta^{(d+1)/2}]Z_1(z,\beta), \tag{10}$$

and from Eqs. (8) and (9) the result follows readily as

$$\rho_d(z)=\frac{k^d}{2^d\pi^{(d+1)/2}\frac{1}{2}\cdot\frac{3}{2}\cdots d/2}$$
$$-\left(\frac{2}{\pi}\right)^{1/2}\frac{1}{(2\pi)^{d/2}}k^d\frac{j_{(d-1)/2}(2kz)}{(2kz)^{(d-1)/2}}. \tag{11}$$

This result (11), valid for d odd, is easily shown to include Eqs. (2) and (5) for the special cases $d=1$ and $d=3$, respectively.

The case of d even can similarly be handled; one merely notes here the result

$$\mathscr{L}(1/\beta)e^{-2z^2/\beta}=K_0(2kz), \tag{12}$$

which enables $\rho_2(z)$, etc. to be calculated in terms of the appropriate Bessel functions of a purely imaginary argument.

II. KINETIC ENERGY DENSITY IN d DIMENSIONS

Returning to the case of d odd, one can also calculate the kinetic energy density. Using the Bloch equation, this is easily written for the case of classical statistics as

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$$t_d^{(c)}(z) = -\frac{\partial Z_d}{\partial \beta} = -\frac{1}{(2\pi\beta)^{(d-1)/2}}\frac{\partial Z_1}{\partial \beta} - \frac{((1-d)/2)Z_1}{(2\pi)^{(d-1)/2}\beta^{(d+1)/2}}. \quad (13)$$

Utilizing the expression for $\partial Z_1/\partial\beta$,

$$\frac{\partial Z_1}{\partial \beta} = -\frac{1}{2(2\pi)^{1/2}\beta^{3/2}} - \frac{2z^2}{(2\pi)^{1/2}} \times \frac{\exp(-2z^2/\beta)}{\beta^{5/2}} + \frac{\exp(-2z^2/\beta)}{2(2\pi)^{1/2}\beta^{3/2}}, \quad (14)$$

one can calculate the degenerate kinetic energy $t_d(z)$ corresponding to the electron density (11) as the inverse Laplace transform of $t_d^{(c)}(z)/\beta$. One then obtains

$$t_d(z) = \frac{1}{2(2\pi)^{d/2}}\mathcal{L}^{-1}\left[\frac{d}{\beta^{(d+4)/2}} - \frac{d\exp(-2z^2/\beta)}{\beta^{(d+4)/2}} + \frac{4z^2\exp(-2z^2/\beta)}{\beta^{(d+6)/2}}\right]. \quad (15)$$

Again utilizing Eqs. (8) and (9), one finds, after a short calculation,

$$t_d(z) = \frac{d}{2\pi^{1/2}(2\pi)^{d/2}\frac{1}{2}\cdot\frac{3}{2}\cdots(d+2)/2}\left(\frac{k^2}{2}\right)^{(d+2)/2} + \frac{k^{d+2}}{2\pi^2(2\pi)^{(d-3)/2}} \times \left[\frac{j_{(d+1)/2}(2kz)}{(2kz)^{(d+1)/2}} - \frac{2j_{(d-1)/2}(2kz)}{(2kz)^{(d-1)/2}}\right], \quad (16)$$

where use has been made of the relations[5]

$$\frac{d}{dx}[x^{-l}j_l(x)] = -x^{-l}j_{l+1}(x) \quad (17)$$

and

$$j_{l-1}(x) + j_{l+1}(x) = (2l+1)/x\, j_l(x). \quad (18)$$

Equation (16) represents the d-dimensional kinetic energy corresponding to the electron density (11). As a final step, it is worth substituting in Eq. (16) for $j_{(d-1)/2}(2kz)$ from Eq. (11), to obtain the desired result

$$t_d(z) = t_{d0} + \frac{k^2}{2}[\rho_d(z) - \rho_{d0}] + \frac{k^{d+2}}{2\pi^2(2\pi)^{(d-3)/2}}\frac{j_{(d+1)/2}(2kz)}{(2kz)^{(d+1)/2}}. \quad (19)$$

In Eq. (19), the first term on the right-hand side is the kinetic energy density of the bulk electron gas. In the second term, $\rho_d(z) - \rho_{(d0)}$ is the charge displaced in the electron gas by the infinite barrier, ρ_{d0} as usual being the bulk density. This term is evidently reflecting the kinetic energy due to adding $\int[\rho_d(z) - \rho_{d0}]d\tau$ electrons at the Fermi energy $k^2/2$. The final term in Eq. (19) is the physically interesting kinetic energy change associated with the induced inhomogeneity of the d-dimensional electron gas. In summary, Eqs. (11) and (17) for the electron density and the corresponding kinetic energy are the main results of this work, both stemming directly from the form (7) of the d-dimensional Slater sum of the noninteracting semi-infinite electron gas. As a by-product of Eq. (11), use of the large z asymptotic form of the spherical Bessel function shows immediately the dimensionality dependence of the long-range oscillations induced in the electron gas by the "perturbing" barrier.

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Topologies for point distributions

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The concepts of void and cluster for an arbitrary point distribution in a domain $\mathscr{D}$ are defined and characterized by some parameters such as volume, density, number of points belonging to them, shape, etc. After assigning a weight to each void and cluster—which is a function of its characteristics—the concept of distance between two point configurations S_1 and S_2 in $\mathscr{D}$ is introduced, both with and without the help of a lattice in the domain $\mathscr{D}$. This defines a topology for the point distributions in $\mathscr{D}$, which is different for the different characterizations of the voids and clusters.

I. INTRODUCTION

The spatial distributions of points in one, two, or a higher number of dimensions (spatial processes, point processes, spatial patterns, spatial point patterns) constitute a very interesting field of research, not only in pure mathematical statistics but also in its innumerable applications, which range from biometrics to astrophysics and includes such diverse fields as agriculture, econometrics, ecology, traffic problems, and medical sciences. In fact, such point distributions may correspond, for instance, to plants of a given species, to cars along a road, to seeds in a field, to microorganisms in a living body, or to stars—or even galaxies or clusters of galaxies—in our Universe. An important mathematical aspect of spatial processes is the study of the geometrical and topological properties of point distributions.

Although in biometry the study of such distributions has always been very popular during the last years—as can be seen through the large number of research articles and even books which have been issued,[1] in the last couple of months the interest about this field of research has grown very rapidly, due in great part to the remarkable discoveries of de Lapparent, Geller, and Huchra about the spatial distribution of galaxies in our Universe.[2] These authors made an optical red shift survey of all 1099 galaxies brighter than magnitude 15.5 of a thin slice of sky and came to the conclusion that galaxies are concentrated on the surfaces of contiguous bubble like structures with very large typical diameters of about 25 h^{-1} Mpc. The large void in Boötes of 60 h^{-1} Mpc, discovered in 1981 by Kirshner *et al.*,[3] has been thereby proved to be no peculiarity but a very common feature. Too often, the analysis of the point distributions of galaxies, with their voids and clusters, is done simply by looking at pictures and plates with the naked eye, a very primitive procedure which in general is not that bad. Nevertheless, the important discoveries we have just mentioned stress once more the necessity for a more profound understanding of spatial point distributions and, in particular, of the still unsolved problem concerning the construction of a mathematical "measure" for quantifying how far away are two of such point distributions (characterized by the number and magnitude of the voids and clusters, their forms and spatial distribution, etc.).

II. DEFINITIONS OF (SPHERICAL) VOID AND CLUSTER

The very large numbers of points one has to deal with makes it almost a necessity to introduce definitions which are suitable to be treated with a numerical algorithm. This has been pointed out in several previous papers on the subject[4] and will be considered later in detail (Sec. VI). However, I do not think that discrete algorithms alone can solve these problems satisfactorily, and it is much better to play at a time both with discrete and with continuous concepts.

Let S be a set of points in a given domain $\mathscr{D}$ of volume V in d-dimensional Euclidean space. Let N be the number of points in S. For any point $p \in \mathscr{D}$ and any positive real number $r \in \mathbb{R}^+$, the density of points in a ball around p of radius r is given by

$$\rho_p(r) = n_p(r)/V_p(r), \tag{2.1}$$

where $n_p(r)$ is the number of points of S inside the ball, and $V_p(r)$ is the volume of the ball. By definition, there is a void around p of radius bigger than r if the density $\rho_p(r)$ verifies

$$\rho_p(r) < \lambda N/V, \tag{2.2}$$

where $\lambda \leqslant 1$ must be fixed (we may take, for instance, $\lambda = \frac{1}{2}$). The radius of the void around p is defined to be the value r_p such that

$$\rho_p(r_p) = \lambda N/V. \tag{2.3}$$

In this way the density of any void will be the same. Alternatively, one could define the radius of the void as the value of r at which the slope of $\rho_p(r)$ is maximum.

On the other hand, there exists, by definition, a cluster around p if

$$\rho_p(r) > N/\lambda V. \tag{2.4}$$

The radius of the cluster may be defined to be the value r_p such that

$$\rho_p(r_p) = N/\lambda V. \tag{2.5}$$

As before, one could alternatively define the radius of the cluster as the value of r at which the slope of $-\rho_p(r)$ is maximum.

Until now we have studied only what happens at some given place p. A global analysis has to distinguish between the different voids and clusters, so that we do not count the

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same point of the distribution twice: as belonging to a void (or cluster) and to another one which intersects the first. Moreover, the preceding definitions are best suited for spherical voids or clusters only and when p is the center of them. These difficulties will be taken care of in the subsequent sections.

III. EFFICIENT SEARCH FOR VOIDS AND CLUSTERS

Let us now introduce a lattice $\mathscr{L}$ of lattice site a in the domain $\mathscr{D}$. For a given set of $r_k \in \mathbb{R}^+$, $k = 1,2,...,m$, select the set S_1 of vertices of the lattice corresponding to the s smallest and to the h highest values of $\rho_{p_i}(r_k)$, for all $k = 1,2,...,m$, for all lattice vertices p_i on $\mathscr{L}$. Improve now the set of points p_i in S_1 to a set S_2 coming from the s smallest and h highest values of $\rho_{q_i}(r_k)$ for all $k = 1,2,...,m$, and for all q_i of the form

$$p_i + \lambda \left[\prod_{k=1}^{m} \rho_{p_i}(r_k) \right]^{-1/2m} \hat{e}, \tag{3.1}$$

where λ is a constant that we can adjust at will (for instance, $\lambda = \frac{1}{2}$ for voids and $\lambda = 2$ for clusters), while $\hat{e}$ sweeps all unitary directions of the form

$$\hat{e}_{i_1} \pm \cdots \pm \hat{e}_{i_l}, \quad 1 \leqslant i_1 < \cdots < i_l \leqslant d, \tag{3.2}$$

where $\hat{e}_i$ is the unitary vector along the i axis of $\mathbb{R}^d$. Notice that, in general, the points q_i are not vertices of the lattice. In fact, the vertices of the lattice serve only as starting points in order to begin the search for the best centers of the voids and clusters.

The procedure is then repeated until it stabilizes. In this way we obtain the positions of the centers of a desired number of the less dense voids and of the more dense clusters in the point distribution S.

IV. WEIGHTS OF THE INDIVIDUAL VOIDS AND CLUSTERS

The weight of a spherical void of radius r and density ρ with the center at the point p is given by the following expression:

$$W_v = k_v [V_p(r)/\rho] = k_v [V_p(r)^2/n], \tag{4.1}$$

where k_v is a constant (independent of the void), $V_p(r)$ the volume of a sphere of radius r in d dimensions, and n is the number of points of S inside the sphere. That this expression is correct can be seen through the following argument. For a given density ρ, increase of W_v in (4.1) is proportional to the volume of the void, while for fixed volume, increase of W_v is proportional to decrease of ρ_i, as it should be by intuition. Alternatively, at fixed n increase of W_v is proportional to the volume and *also* to the decrease of density, i.e., proportional to the volume squared.

The weight of a spherical cluster of radius r and density ρ centered at p is given by

$$W_c = k_c n\rho = k_c [n^2/V_p(r)] = k_c \rho^2 V_p(r), \tag{4.2}$$

where k_c is a constant independent of the cluster. Expression (4.2) can be understood by reasoning as follows. At fixed n, W_c is proportional to increase of ρ (or to decrease of volume). At fixed ρ, W_c is proportional to increase of n (or to increase of volume). Alternatively, with full generality, increase of W_c is due both to increase of n (it would also be true for fixed ρ, i.e., letting volume increase) and to increase of ρ.

V. THE SET OF ALL POINT DISTRIBUTIONS AS A METRIC SPACE

Once the spherical voids and clusters have been constructed by the procedures described in Secs. II and III, and just before their individual weights (Sec. IV) are calculated, one has to look for superpositions of them which may result in nonspherical voids and clusters. The idea is very simple: to consider as a unique void (resp. cluster) the union of all of them which are connected by a chain of intersections (Fig. 1). In this way, the numbers of voids and clusters, s and h, respectively, diminish and, at the same time, they are no more spherical but acquire a form of the type depicted in Fig. 2. It is now immediate to modify the formulas (4.1) and (4.2) accordingly: in both cases the volume $V_p(r)$ of a d-dimensional sphere of radius r centered at p must be substituted by the volume of the void or cluster considered. Of course, the density ρ and the number of points n will also correspond now to the whole, nonspherical void or cluster.

Once all the voids and all the clusters have been constructed, the remaining region of the domain $\mathscr{D}$ is filled up with a (under ideal conditions) sensibly uniform distribution of points of S with a density almost equal to $\rho_0 = N/V$. In practice this must be checked *a posteriori* and if it were not true, the free parameters introduced in the definitions and construction of the voids and clusters (s, h,...) ought to be changed accordingly. For instance, if the density of the remaining region were smaller than ρ_0, then the number s of voids should be increased. On the other hand, if the homogeneity of the remaining region were not very good then both s and h ought to be augmented.

Let us now consider the plane (V,ρ) and the points (V_i,ρ_i) in it, where the index i goes through all the different voids and clusters, with one value of the index corresponding to the intermediate, remaining region. Introduce a regular lattice in this plane and denote the different cells by (V_j,ρ_j), $j \in \mathscr{J}$. Define now the function $f(V_j,\rho_j)$ which as-

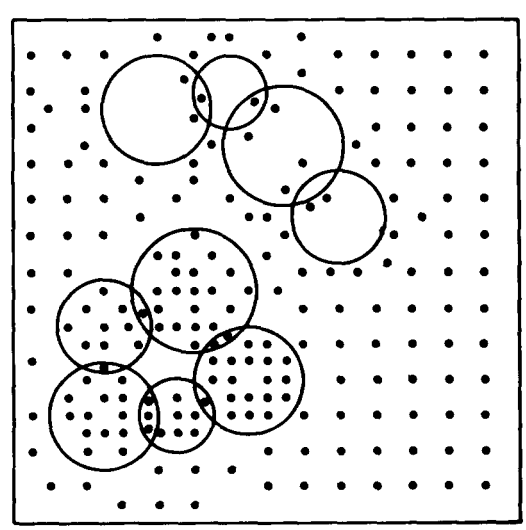

FIG. 1. Examples for distributions of spherical voids and clusters. They can superpose in a variety of ways.

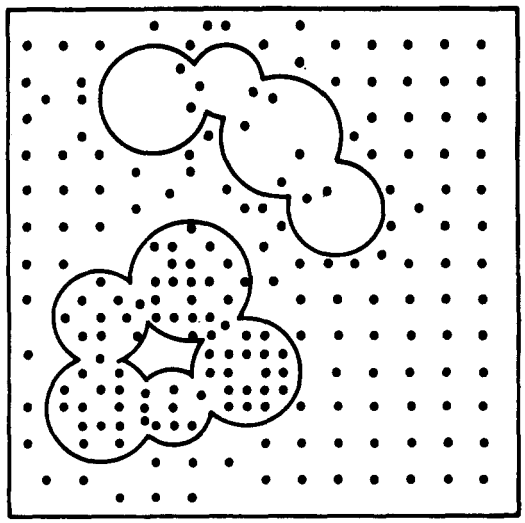

FIG. 2. Voids and clusters constructed from the distributions of Fig. 1 in order to avoid overcounting.

signs to each cell (V_j,ρ_j) the number of clusters plus the number of voids which belong to this cell, each of them multiplied by the corresponding weight (4.2) and (4.1), respectively, i.e.,

$$f(V_j,\rho_j) = n_c(V_j,\rho_j)W_c(V_j,\rho_j) + n_v(V_j,\rho_j)W_v(V_j,\rho_j), \quad j\in\mathscr{J}. \tag{5.1}$$

Here the intermediate region is to be counted as an additional void or cluster depending on its density ρ being $\rho\leqslant\rho_0$ or $\rho>\rho_0$, respectively. Notice that $f(V_j,\rho_j)$ is different from zero only in a finite number of cells (V_j,ρ_j). The following step is to construct with these points the minimal triangulated surface with vertices at these points. Thus, we get a continuous function $f(V,\rho)$ defined on the plane (V,ρ). Now, given another point configuration on the domain $\mathscr{D}$, we define the distance between these two configurations S_1 and S_2 by

$$d(S_1,S_2)^2 = \iint [f_1(V,\rho) - f_2(V,\rho)]^2\, dV\, d\rho, \tag{5.2}$$

where f_1 and f_2 are the functions corresponding to the point configurations S_1 and S_2, respectively.

The problem we are dealing with is not so standard. No wonder, therefore, that definition (5.2) is not a *usual* measure of the configuration space. However, it is important to observe that d, as given by (5.2), can be easily implemented to yield a true distance by the usual mathematical procedures. Let us be completely rigorous.

The set which is going to turn into a metric space is $\mathscr{S}$ = set of all finite point distributions in the domain $\mathscr{D}$. The "distance" defined by (5.2) is actually only a semidistance. In fact, it satisfies (i) $d(S_1,S_2)=0$, (ii) $d(S_2,S_1)=d(S_1,S_2)$, and (iii) $d(S_1,S_2)\leqslant d(S_1,S_3)+d(S_3,S_2)$, for any $S_1,S_2,S_3\in\mathscr{S}$. All we have to do is to define the coset $\bar{\mathscr{S}}=\mathscr{S}/\sim$, where $S_1\sim S_2$ iff $d(S_1,S_2)=0$, in order to obtain a metric space $\bar{\mathscr{S}}$ with the distance $\bar{d}$ given by

$$\bar{d}(\bar{S}_1,\bar{S}_2) = d(S_1,S_2),\ S_1\in\bar{S}_1,\ S_2\in\bar{S}_2. \tag{5.3}$$

In fact, this is a consistent definition for, let us consider two other configurations $S_1'\in\bar{S}_1$ and $S_2'\in\bar{S}_2$. Then, we have

$$d(S_1,S_2)\leqslant d(S_1,S_1') + d(S_1',S_2') + d(S_2',S_2).$$

But $d(S_1,S_1')=0$ and $d(S_2,S_2')=0$, so that $d(S_1,S_2)\leqslant d(S_1',S_2')$. Moreover,

$$d(S_1',S_2')\leqslant d(S_1',S_1) + d(S_1,S_2) + d(S_2,S_2'),$$

and we get $d(S_1',S_2')\leqslant d(S_1,S_2)$. Therefore, $d(S_1',S_2')=d(S_1,S_2)$. Equation (5.3) defines a distance $\bar{d}$ on $\bar{\mathscr{S}}$. In fact, $\bar{d}$ satisfies the axioms (i)–(iii) above and, moveover, the additional one, (i') $\bar{d}(\bar{S}_1,\bar{S}_2)=0$ implies $\bar{S}_1=\bar{S}_2$. This is immediate from (5.3) and from the definition of the coset $\bar{\mathscr{S}}$.

Summing up, $\bar{\mathscr{S}}$ is a metric space endowed with the distance $\bar{d}$. This constructive procedure is very well known to mathematicians, in fact, it is the standard way to proceed. This allows one to be a little loosely in the notation and speak of the metric space $\mathscr{S}$ and of the distance d, as given by (5.2). The alternative definitions of distance which will follow have to be compared with (5.2). Actually all of them ought to be submitted to the same procedure as given above in order that they become true distances $\bar{d}$.

A metric space is readily made into a topological space, the topology being provided by the distance, much as in the standard example of the metric space $\mathbb{R}^n$. The neighborhoods of the basis of this topology are open balls of the form $B_p(\bar{S}) = \{\bar{S}'\in\bar{\mathscr{S}} \mid \bar{d}(\bar{S},\bar{S}')<p\}$, p being any rational number $p\in\mathbb{Q}$. Being again a little loosely with the notation we may say that the set $\mathscr{S}$ of all finite point distributions in $\mathscr{D}$ is a topological space, the topology being given through the distance d in (5.2).

This is by no means the only possibility to define a distance between two point configurations. But the definition which has just been given above is quite a sensible one. An example of a different, more simple definition is the following. Consider the weights (4.1) and (4.2) and place them at the negative and positive semiaxis x, respectively (Fig. 3). Then discretize this axis by considering intervals of a given length l. For each interval of the x axis, on the y axis set the number of voids (resp. clusters) with a value of W_v (resp. W_c) which belongs to this interval. Now consider the segment-wise curve constructed with the resulting points (Fig. 3). Let us call this curve $g(x)$. The distance between two point configurations S_1 and S_2 can then by defined by

$$d(S_1,S_2)^2 = \int [g_1(x) - g_2(x)]^2\, dx. \tag{5.4}$$

Notice, however, that on taking the weights from the beginning we have implicitly introduced in this last case an equivalence relation among voids (and among clusters). In some cases this can actually be convenient in order to simplify the problem from the beginning, but in other situations a finer definition such as the first one will have to be adopted.

VI. POINT DISTRIBUTIONS IN A DOMAIN WITH A LATTICE

In order to treat all the preceding questions in a way better suited for numerical manipulations, one can carry all these definitions to a lattice $\mathscr{L}$ of certain site a on the do-

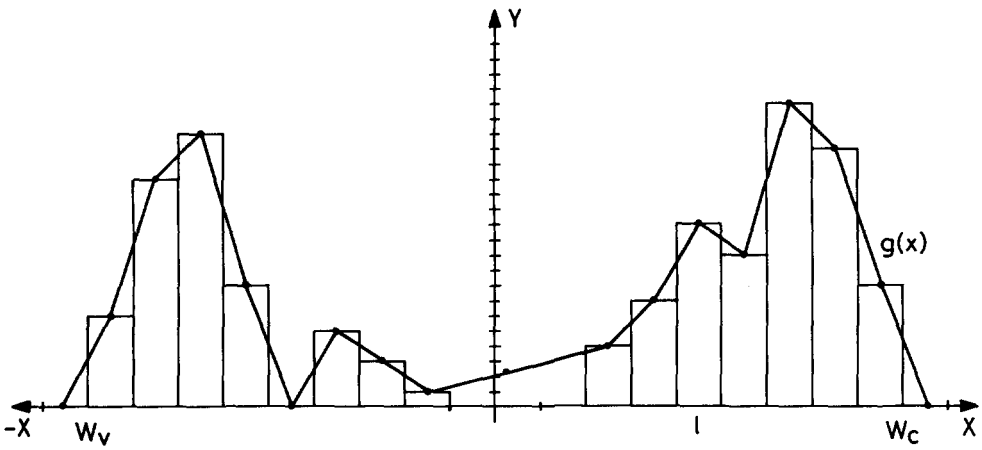

FIG. 3. Segment-wise curve $g(x)$ constructed using a discretization of the weights corresponding to voids (negative x axis) and clusters (positive x axis). In the y axis the numbers of voids and clusters that fall into each interval of x are represented.

main $\mathscr{D}$. That is, a discretization of the methods which have been elaborated above has to be developed.

One must start by counting the number of points of the distribution S in $\mathscr{D}$ that fall into each of the elementary cells of the lattice. The voids will consist of all those cells whose number of points does not reach a value n_1 fixed in advance, while the clusters are made up of cells with a number of points above a second number n_2 also fixed in advance. Of course, one must have

$$n_1 < N/N_c < n_2, \tag{6.1}$$

where $N_c = V/a^d$ is the number of cells of the lattice $\mathscr{L}$. (To begin with, we consider all cells equal and obviate the small modifications in these definitions which had to be made for cells touching the border of the domain $\mathscr{D}$.) In this way, extended voids and clusters made up of cells will arise, in general. A huge void (cluster) will consist of several contiguous cells with a small (big) number of points. Figure 2 will be almost the same, only that the curved contour will be substituted by a segment-wise one, with segments of longitude proportional to a. Formulas (4.1) and (4.2) will remain unchanged: only $V_p(r)$ will be substituted by the volume V_v or V_c of the void or cluster under consideration (a volume always proportional to a^d, the volume of an elementary cell).

Notice that this procedure is less time consuming than the former one when it is carried out in practice. However, it is not so sensible to detect the voids and clusters with precision. In fact, once the lattice $\mathscr{L}$ has been fixed, a given cell can participate at the same time of a void and of a cluster so that the total number of points in it may compensate (Fig. 4), thus hiding this fact completely. Clearly, everything becomes better as a is made smaller (continuum limit). However, with a (discrete) point distribution this cannot be done indefinitely: for a small enough every cell contains at most one point only and for such small cells the whole procedure ceases to be of much use (this was the difficulty with the topology of discrete point distributions in the first place).

Once the weights (4.1) and (4.2) have been adapted to the lattice voids and clusters, the definitions (5.2)–(5.4) for the distance between two point configurations S_1 and S_2 go through immediately. Thus, we complete the treatment of the lattice case and define a topology for point configurations on the domain $\mathscr{D}$. One could think, in principle, that in order to proceed in accordance with the discretization of $\mathscr{D}$, the plane (V,ρ) ought also to be discretized, i.e., divided into rectangles of sides a_V and a_ρ, and the minimal triangulated surfaces constructed using the vertices corresponding to the centers of these cells. However, it must be pointed out that this last discretization is completely independent from the one of the domain $\mathscr{D}$.

Finally, notice that in our definition only the volume and the density (we may substitute one of these by the number of points inside) of the void or cluster have been taken into account in the definition of the distance $d(S_1,S_2)$. A more elaborate definition should also include other parameters such as some characterizing the shape of the void or cluster (for instance, a combination of the diameters along each of the axes, as the sum or the product of these diameters). The function $f(V,\rho)$ given in (5.1) and the distance (5.2) have to be redefined accordingly. That is (we drop the subindex j for convenience)

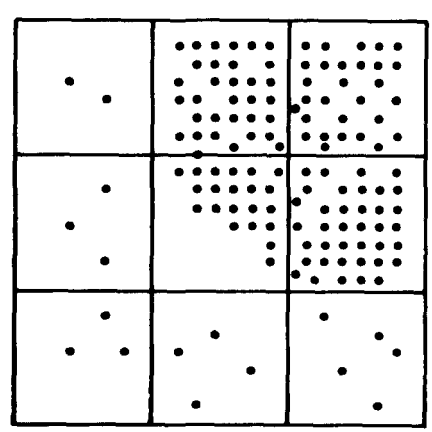

FIG. 4. Some cells (here the one in the middle) of a lattice in $\mathscr{D}$ may participate both from some void and from some cluster. They may compensate and give a deceptive mean density approximately equal to $\rho_0 = N/V$.

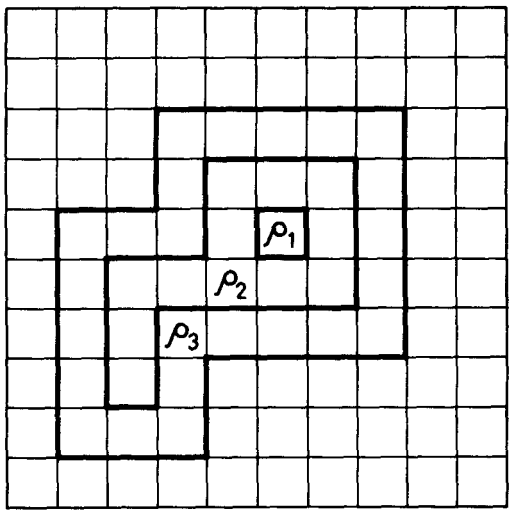

FIG. 5. A huge void or cluster (the points have not been depicted) displaying the gradient of density: ρ_1 is the density of the most inner cell; ρ_2 that of the surrounding crown of cells (here 12 cells); ρ_3 is the density of the most exterior crown (here 24 cells).

$$f(V,\rho,k) = n_c(V,\rho,k)\,W_c(V,\rho,k) - n_v(V,\rho,k)\,W_v(V,\rho,k), \tag{6.2}$$

where k is the new parameter, and

$$d(S_1,S_2)^2 = \iiint [f_1(V,\rho,k) - f_2(V,\rho,k)]^2\, dV\, d\rho\, dk, \tag{6.3}$$

respectively. In an analogous way, we may introduce other parameters, such as the gradient of density for large voids or clusters, as one proceeds from inside to the border (Fig. 5). We may define, for instance,

$$h = [(\rho_2 - \rho_1)^2 + (\rho_3 - \rho_2)^2 + \cdots]^{1/2} \tag{6.4}$$

and include h besides k as a new parameter. All these parameters and others one may think of improve the definition of the topology (6.3) and may be introduced at ease into our formalism in the way we have just shown.

VII. OUTLOOK

The procedures introduced here for the first time (to our knowledge) are currently being applied to the point distributions that correspond to the analysis of galaxies of de Lapparent *et al.*[2] and also to other related results. Moreover, simulation methods are being developed with the purpose of checking the reliability of the distance between point distributions as defined here compared with the only one which is presently available, namely, the "distance" that our naked eye would *grosso modo* assign to them. The investigation is in progress. Its partial results are pretty good and will be published elsewhere with a detailed account of the analysis involved.

ACKNOWLEDGMENTS

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Comment on "On a property of a classical solution of the nonlinear mass transport equation $u_t = u_{xx}/1 + u_x^2$. II" [J. Math. Phys. 28, 536 (1987)]

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A mechanism of smoothing due to evaporation condensation of the roughly perturbed surface of a solid is formulated as a Cauchy problem in the real line $\mathbb{R}^1$ for the equation $u_t = u_{xx}/1 + u_x^2$, which describes the evolution of the profile $u(x,t)$ of the surface. In the preceding paper [A. Kitada and H. Umehara, J. Math. Phys. **28**, 536 (1987)], it was demonstrated that, if the solution $u(x,t)$ of the Cauchy problem is obtained in the classical sense with an additional restriction $u \in C^3(\mathbb{R}^1 \times (0,\infty))$, each peak in the surface decreases in height with time in the strict sense. In the present paper, by modifying the proof, it is shown that the additional restriction to the classical solution is excessive.

I. INTRODUCTION

In the preceding paper,[1] using the maximum principle due to Nierenberg,[2] well known in the theory of linear parabolic equations, we obtained the estimate (1),

$$u(x_2,t_2) < u(x_1,t_1), \quad (x_i,t_i) \in C \quad (i=1,2), \quad t_1 < t_2, \qquad (1)$$

describing the strictly monotone decrease with time t, due to evaporation condensation, in the height of a peak in a roughly perturbed surface of solid. In the estimate (1), $u(x,t)$ is such a classical solution[3] that $u \in C^3(\mathbb{R}^1 \times (0,\infty))$ (Ref. 4) of the Mullins' model (P) (Ref. 5) in the real line $\mathbb{R}^1$,

$$\begin{aligned} &u_t = u_{xx}/1 + u_x^2, \quad (x,t) \in \mathbb{R}^1 \times (0,\infty), \\ &u(x,0) = \alpha(x), \quad x \in \mathbb{R}^1, \end{aligned} \qquad (P)$$

and C is a trajectory in the (x,t) plane drawn by the migration with time of a peak top in $\alpha(x)$; that is, the set C is characterized by

$$C = \{(x,t); x = g(t), g \in C^1([0,t_f])\}, \qquad (2a)$$

$$u_x(x,t) = 0, \quad u_{xx}(x,t) < 0, \quad (x,t) \in C. \qquad (2b)$$

In the present paper, we show that the estimate (1) holds for the ordinary classical solution of the problem (P) without the additional restriction $u \in C^3(\mathbb{R}^1 \times (0,\infty))$; that is, the restriction $u \in C^3(\mathbb{R}^1 \times (0,\infty))$ is shown to be excessive.

II. A DEMONSTRATION OF THE STRICTLY MONOTONE DECREASE IN HEIGHT OF A PEAK IN THE CLASSICAL SOLUTION

We will make general discussions on the following Cauchy problem (P*) which is a generalization of the Mullins' model (P):

$$\begin{aligned} &u_t = F(u_x, u_{xx}), \\ &[F \in C^1(\mathbb{R}^2),\ F_q(p,q) > 0 \text{ (Ref. 6)}, F(0,0) = 0], \\ &(x,t) \in \mathbb{R}^1 \times (0,\infty), \\ &u(x,0) = \alpha(x), \quad x \in \mathbb{R}^1. \end{aligned} \qquad (P^*)$$

As is pointed out in our previous paper,[7] the solution of (P*) must satisfy the following problem (LP):

$$\begin{aligned} &u_t - u_{xx} \int_0^1 F_q(hu_x(x,t), hu_{xx}(x,t))dh \\ &\quad - u_x \int_0^1 F_p(hu_x(x,t), hu_{xx}(x,t))dh = 0, \\ &(x,t) \in \mathbb{R}^1 \times (0,\infty), \\ &u(x,0) = \alpha(x), \quad x \in \mathbb{R}^1, \end{aligned} \qquad (LP)$$

where the function $F(p,q)$ is what is given in the problem (P*). In the preceding paper,[1] we showed that if the maximum principle due to Nierenberg is applicable to the problem (LP), the estimate (1) holds, and in order for the maximum principle to be applicable to (LP), it is sufficient that all the coefficients of the linear equation in (LP) are continuous at any point of the set $\mathbb{R}^1 \times (0,\infty)$. In the preceding paper,[1] we used the mean value theorem in the differential calculus to show the continuity of the coefficients

$$\int_0^1 F_q(hu_x(x,t), hu_{xx}(x,t))dh$$

and

$$\int_0^1 F_p(hu_x(x,t), hu_{xx}(x,t))dh.$$

In this context, the additional restriction $u \in C^3(\mathbb{R}^1 \times (0,\infty))$ was required.[8] In the present paper, we replace the procedure of the demonstration by the following one which does not require this restriction.

Proof of the continuity of the coefficients: We will show the continuity of the coefficient of u_{xx},

$$\int_0^1 F_q(hu_x(x,t), hu_{xx}(x,t))dh,$$

at the arbitrarily fixed point $(x_0,t_0) \in \mathbb{R}^1 \times (0,\infty)$. Let Ω be a bounded open convex set in the real plane $\mathbb{R}^2$, for example, an open disk, which contains two points (p_0,q_0) and $(0,0)$. Here, $p_0 = u_x(x_0,t_0)$ and $q_0 = u_{xx}(x_0,t_0)$. Since the closure of Ω, $\bar{\Omega}$, is compact and the function $F_q(p,q)$ is continuous as is indicated in (P*), $F_q(p,q)$ is uniformly continuous on $\bar{\Omega}$. Therefore, for any $\epsilon > 0$, there exists $\delta > 0$ such that

$$\begin{aligned} &|F_q(hp,hq) - F_q(hp',hq')| \\ &\quad < \epsilon [0 \leqslant h \leqslant 1,\ (p,q) \in \bar{\Omega},\ (p',q') \in \bar{\Omega}], \end{aligned}$$

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whenever $|p-p'|<\delta$ and $|q-q'|<\delta$. As both functions $u_x(x,t)$ and $u_{xx}(x,t)$ are continuous at the point (x_0,t_0), for the above $\delta>0$, there exists $\eta>0$ such that

$$|u_x(x,t)-u_x(x_0,t_0)|<\delta, \quad |u_{xx}(x,t)-u_{xx}(x_0,t_0)|<\delta,$$

whenever $|x-x_0|<\eta$ and $|t-t_0|<\eta$. Combining the above two estimates, we have

$$\begin{aligned}&\left|\int_0^1 F_q(hu_x(x,t),hu_{xx}(x,t))dh\right.\\&\quad\left.-\int_0^1 F_q(hu_x(x_0,t_0),hu_{xx}(x_0,t_0))dh\right|\\&\quad\leqslant\int_0^1 |F_q(hu_x(x,t),hu_{xx}(x,t))\\&\qquad-F_q(hu_x(x_0,t_0),hu_{xx}(x_0,t_0))|dh<\epsilon,\end{aligned}$$

for any (x,t) such that $|x-x_0|<\eta$ and $|t-t_0|<\eta$. This means the continuity of the coefficient of u_{xx} at the point (x_0,t_0). As the same is true for the coefficient of u_x, all the coefficients of the linear equation in (LP) are continuous. □

We can conclude that the estimate (1) holds for the classical solution without the restriction $u\in C^3(\mathbb{R}^1\times(0,\infty))$.

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[1] A. Kitada and H. Umehara, J. Math. Phys. **28**, 536 (1987).

[2] L. Nirenberg, Commun. Pure. Appl. Math. **6**, 167 (1956).

[3] O. A. Ladyzenskaja, V. A. Solonikov, and N. N. Ural'ceva, *Linear and Quasilinear Equations of Parabolic Type* (Am. Math. Soc., Providence, RI, 1968), p. 12.

[4] The symbol $C^m(\Omega)$ denotes the set of all functions defined on Ω whose partial derivatives of order $\leqslant m$ are all continuous.

[5] W. W. Mullins, J. Appl. Phys. **28**, 333 (1957); **30**, 77 (1959).

[6] The partial derivative $\partial F/\partial q$ is abbreviated as F_q. In the same manner, we write $\partial F/\partial p$ as F_p.

[7] A. Kitada, J. Math. Phys. **27**, 1391 (1986).

[8] Moreover, in the preceding paper,[1] the extent of the generalization (P*) of the Mullins' model was also limited by the excess restriction $F\in C^2(\mathbf{R}^2)$. In the present paper, this restriction is so softened as $F\in C^1(\mathbf{R}^2)$.

Relativistic Coulomb Sturmian matrix elements and the Coulomb Green's function of the second-order Dirac equation

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Matrix elements with respect to a discrete "Sturmian" basis set of the operator $r^{1/2}gr^{1/2}$, where g is the Coulomb Green's function of the "second-order" Dirac equation, are investigated. Closed expressions, involving Gaussian hypergeometric functions, can be obtained for the matrix elements. This calculation illustrates contour integration techniques capable of yielding closed expressions for a number of overlap integrals associated with the relativistic Kepler problem.

I. INTRODUCTION

Discrete Coulomb Sturmian basis sets have been used successfully for some time in nonrelativistic atomic calculations.[1] One of the first examples of a Sturmian basis set appeared in a discrete expansion of the nonrelativistic Coulomb Green's function in momentum space due to Schwinger.[2] Sturmian functions in this discrete expansion entered as a set of four-dimensional spherical harmnics connected with the O(4) symmetry of the nonrelativistic Kepler problem. A coordinate space form of Schwinger's expansion was investigated in which the Sturmian functions arose in a different way as "coupling constant eigenfunctions."[3] Subsequently, it was found that the coupling constant eigenfunction concept could yield a discrete expansion also for the relativistic Coulomb Green's functions. The Coulomb Green's functions for both the "second-order" Dirac equation[4] (defined below) and the conventional linear Dirac equation[5] have been studied from this point of view.

The Sturmian basis sets seem convenient for atomic calculations, since through the use of the Sturmian basis sets one can avoid the introduction of continuum states, and this without sacrificing completeness. In perturbation calculations using a Coulomb Sturmian basis set there will in general be a need for Sturmian matrix elements of the Coulomb Green's function. Such matrix elements will be investigated here for the second-order Dirac equation,

$$\{\Pi\cdot(1+i\sigma)\cdot\Pi+m^2\}\Phi=0,\qquad \Pi_\mu\equiv -i\,\partial_\mu - eA_\mu, \tag{1.1}$$

in which the wave function Φ is a 2×1 Pauli spinor, and $\sigma_{\mu\nu}$ is a self-dual Lorentz spin tensor, defined by the equation

$$\sigma_{\mu\nu}\equiv\left[\begin{array}{ccc|c} 0 & \sigma_3 & -\sigma_2 & \sigma_1 \\ -\sigma_3 & 0 & \sigma_1 & \sigma_2 \\ \sigma_2 & -\sigma_1 & 0 & \sigma_3 \\ \hline -\sigma_1 & -\sigma_2 & -\sigma_3 & 0 \end{array}\right], \tag{1.2}$$

$\sigma_{1,2,3}$ being the ordinary 2×2 Pauli spin matrices. Equation (1.1) has been discussed by a number of authors[4,6–18] and is known to be equivalent to the usual linear Dirac equation. The second-order Dirac equation (1.1) brings out a close parallel between the quantum theory of a Dirac particle and the quantum theory of a simple scalar particle. For this reason, and because of the small dimension of the matrices involved, calculations in quantum electrodynamics are expected to simplify when the second-order form of the Dirac equation is used. These expectations have been borne out in a recent study of the mass operator for an electron in an external Coulomb potential.[19]

To carry the study of the mass operator referred to above further and turn it into a new Lamb shift calculation, matrix elements with respect to a Sturmian basis set of the Coulomb Green's function of the second-order Dirac equation are required. Since these matrix elements will be useful, in general, for a variety of perturbation calculations, it was decided to publish the investigation of the matrix elements of the Green's function separately. The results presented here generalize known results for the nonrelativistic Coulomb Green's function.[20] Also, this calculation illustrates contour integration techniques capable of yielding closed expressions for a number of overlap integrals associated with the relativistic Kepler problem.

In Sec. II the relativistic Coulomb Sturmian basis sets are discussed and the derivation of the overlap integral between two different such basis sets is indicated. Although this material is not especially new, the derivation of the overlap integral is considered because some intermediate steps in the derivation provide a point of departure for the later work with the Coulomb Green's function. The Coulomb Green's function material is presented in Sec. III. Armed with the contour integration technique used for the overlap integral, it is shown how to obtain a closed analytic expression, involving Gaussian hypergeometric functions, for the operator $r^{1/2}gr^{1/2}$, where g is the Coulomb Green's function of the second-order Dirac equation. The factors $r^{1/2}$ supplied on each side of the Green's function before taking matrix elements are essential to obtain this relatively simple result. Because of these factors, the most difficult integrals encountered in Sec. III are of the Gaussian hypergeometric type.

Sturmian basis sets and the Coulomb Green's function of the second-order Dirac equation are discussed in detail in the literature cited above. In the interest of brevity the reader is referred to this earlier work, especially Ref. 4, for background material.

II. COULOMB STURMIAN BASIS SETS

The reader will find a more heuristic introduction to Sturmian basis sets in the literature cited above. Here a pure-

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ly mathematical approach seems best. Relativistic Coulomb Sturmian functions will be defined as the eigenfunctions of the self-adjoint operator

$$O \equiv \left[\frac{r}{2}\right]^{1/2}\left[-\frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r} + \eta^2 - \frac{1-(2\gamma+1)^2}{4r^2}\right]\left[\frac{r}{2}\right]^{1/2} \tag{2.1}$$

acting on the space of spinor functions $\Phi(\mathbf{r})$. Here $\eta > 0$ is an arbitrary real constant, and γ is a self-adjoint operator acting on only the angular and spin degrees of freedom of $\Phi(\mathbf{r})$ and having the eigenvalues $\gamma = [(J+\frac{1}{2})^2 - (Z\alpha)^2]^{1/2}$ if $L = J + \frac{1}{2}$, and $\gamma = [(J+\frac{1}{2})^2 - (Z\alpha)^2]^{1/2} - 1$ if $L = J - \frac{1}{2}$. The corresponding eigenfunctions $\langle \mathbf{r}|\eta,n,L,J,M\rangle$ form a discrete basis. These eigenfunctions are proportional to the spinor spherical harmonics $Y_{LJM}(\mathbf{r})$:

$$\langle \mathbf{r}|\eta,n,L,J,M\rangle = \langle r|\,|\eta,n,L,J\rangle Y_{LJM}(\mathbf{r}), \tag{2.2}$$

$$\langle r|\,|\eta,n,L,J\rangle = (2\eta)^{3/2}[(n-1)!/(n+2\gamma)!]^{1/2} \times (2\eta r)^{\gamma-(1/2)}e^{-\eta r}L_{n-1}^{2\gamma+1}(2\eta r). \tag{2.3}$$

The corresponding eigenvalues of O are $O' = \eta(\gamma + n)$. The double bar notation $\langle r|\,|\eta,nL,J\rangle$ is used to signify the radial part of the wave function of the particle. The radial function $\langle r|\,|\eta,n,L,J\rangle$ is without spinor structure. The angular momentum quantum numbers L, J, M are the familiar ones, and n runs over the range 1,2,3,..., independently of the other quantum numbers. The Sturmian functions (2.2) obey the orthogonality and completeness relations $\langle \eta,A\,|\eta,B\rangle = \delta_{A,B}$, $1 = \Sigma_A\,|\eta,A\rangle\langle\eta,A\,|$. Here and subsequently when convenient the shorthand notation A, B, etc. is used to signify the whole set of quantum numbers n, L, J, M.

In applications the Coulomb Sturmian functions (2.2) are needed sometimes with one, sometimes with another value of η. Accordingly, the overlap integral[19]

$$\langle \eta_0,A\,|\,|\eta,B\rangle = \langle \eta,B\,|\,|\eta_0 A\rangle \equiv \int_0^\infty r^2\,dr\langle\eta_0,A\,|\,|r\rangle\langle r|\,|\eta,B\rangle$$
$$= (-1)^{n-1}\left[\frac{(n_>+2\gamma)!}{(n_>-1)!}\frac{(n_<+2\gamma)!}{(n_<-1)!}\right]^{1/2}\frac{(2\zeta-\zeta^2)^{\gamma+1}}{(2\gamma+1)!}(1-\zeta)^{n_>-n_<} \times {}_2F_1(-(n_<-1),2\gamma+1+n_>,2\gamma+2;2\zeta-\zeta^2), \tag{2.4}$$

is sometimes encountered. In Eq. (2.4) $n_> \equiv \max(n_A = n_0, n_B \equiv n)$, $n_< \equiv \max(n_A, n_B)$, and ζ is the parameter

$$\zeta \equiv 2\eta_0/(\eta+\eta_0). \tag{2.5}$$

The contour integration technique needed in Sec. III will be illustrated here in a simpler context by indicating the derivation of the overlap integral (2.4). Also, the first steps in this derivation provide the starting point for the more involved calculation of Sec. III. As noted in the Introduction, the final result, Eq. (2.4), of this section is not new.

Proceeding with the derivation of the overlap integral (2.4), the Laguerre polynomials under the integral sign are replaced using the integral representation[21]

$$L_n^\mu(z) = \frac{1}{2\pi i}\oint_{(0+)} dt\,e^{-tz}\frac{(1+t)^{n+\mu}}{t^{n+1}}. \tag{2.6}$$

The r integral then goes over into a special case of the formula

$$\int_0^\infty dr\,r^{\nu-1}e^{-ar} = \frac{\Gamma(\nu)}{a^\nu}, \quad \mathrm{Re}(\nu)>0, \quad \mathrm{Re}(a)>0, \quad |\arg(a)|<\pi/2. \tag{2.7}$$

At this point the formula

$$\langle \eta_0,n_0|\,|\eta,n_0\rangle = \left[\frac{2\eta_0}{2\eta}\right]^{\gamma+1}\left[\frac{(n_0-1)!(2\gamma+1)!}{(n_0+2\gamma)!}\right]^{1/2} \times\left[\frac{(n-1)!(2\gamma+1)!}{(n+2\gamma)!}\right]^{1/2}$$
$$\times\frac{1}{2\pi i}\oint_{(0+)} du\,\frac{(1+u)^{n_0+2\gamma}}{u^{n_0}} \times\frac{1}{2\pi i}\oint_{(0+)} dw\,\frac{(1+w)^{n+2\gamma}}{w^n}\frac{1}{(w-w_p)^{2\gamma+2}},$$
$$w_p \equiv -\frac{\eta+\eta_0+u2\eta_0}{2\eta}, \tag{2.8}$$

is obtained. In order to obtain the formula (2.8) the convergence condition $\eta + \eta_0 + 2\eta_0\,\mathrm{Re}(u) + 2\eta\,\mathrm{Re}(w) > 0$, corresponding to $\mathrm{Re}(a) \geqslant 0$ in Eq. (2.7), is requried to allow performing the r integral first. Since $\eta + \eta_0 > 0$, this inequality can be arranged simply by taking the loop $(0+)$ about the origins in the u and w planes sufficiently small. The convergence condition then implies that $\eta + \eta_0 + 2\eta_0\,\mathrm{Re}(u) > -2\eta\,\mathrm{Re}(w)$, $-(\eta+\eta_0+2\eta_0\,\mathrm{Re}(u)) < 2\eta\,\mathrm{Re}(w)$, or $\mathrm{Re}(w_p) < \mathrm{Re}(w)$ for all w on the contour of integration. If follows that the singular point w_p in the integrand of the w integral in Eq. (2.8) lies outside the integration contour, when the contours are chosen so as to permit performing the r integral first.

The next step is to perform the w integral. This is facilitated by the fact that the sum of the exponents in the integrand is equal to minus two, $(n+2\gamma)+(-n)+(-(2\gamma+2)) = -2$. Such an integral is said to be of the Gaussian hypergeometric type. For an integral of the Gaussian hypergeometric type a linear transformation $w \equiv (At+B)/(Ct+D)$ can be performed and the transformed integral will have the same general structure as the original integral, having the same number of factors, each of which has the same exponent as before the transformation.[22] For example, to the factor $(w-w_p)^{-(2\gamma+2)}$ of the original

integral, there will correspond a factor proportional to $(t-t_p)^{(2\gamma+2)}$ in the transformed integral, where t_p is the image of w_p. It is true that powers of a new factor $(Ct+D)$ are introduced by the transformation, but for an integral of the Gaussian hypergeometric type the sum of all powers of $(Ct+D)$ that are introduced by the transformation just cancels a corresponding contribution from the Jacobian dw/dt. This "covariance" property of a Gaussian hypergeometric integral under linear transformations can be used to eliminate a particular factor of the integrand, thereby greatly simplifying the integral. This is accomplished for the factor $(w-w_p)^{-(2\gamma+2)}$ in Eq. (2.8) by mapping the point w_p onto the point at infinity, $t_p=\infty$. The linear transformation needed for this is

$$w = tw_p/(t+1+w_p)\,. \tag{2.9}$$

The t plane is mapped into the w plane in such a way that the points $0, -1, w_p$ in the w plane go over into corresponding points in the t plane as follows:

$$\begin{array}{cccc} w=0 & w=-1 & w=w_p \\ \downarrow & \downarrow & \downarrow \\ t=0 & t=-1 & t=\infty \end{array}\,. \tag{2.10}$$

Accordingly, the w integral takes the form

$$\begin{aligned} &\frac{1}{2\pi i}\oint_{(0+)} dw\,\frac{(1+w)^{n+2\gamma}}{w^n}\,\frac{1}{(w-w_p)^{2\gamma+2}} \\ &\quad=(-1)^{n-1}\frac{(1+w_p)^{n-1}}{(-w_p)^{n+2\gamma+1}}\,\frac{1}{2\pi i} \\ &\qquad\times\oint_{(0+)} dt\frac{(1+t)^{n+2\gamma}}{t^n} \\ &\quad=(-1)^{n-1}\frac{(1+w_p)^{n-1}}{(-w_p)^{n+2\gamma+1}}\,\frac{(n+2\gamma)!}{(n-1)!(2\gamma+1)!}, \end{aligned} \tag{2.11}$$

when transformed into the t plane. The final t integral in Eq. (2.11) was evaluated by use of the following integral representation of a binomial coefficient:

$$(2\pi i)^{-1}\oint dt(1+t)^{n+2\gamma}t^{-n}=\frac{(n+2\gamma)!}{(n-1)!(2\gamma+1)!}\,. \tag{2.12}$$

When the final result (2.11) for the w integral is substituted into the expression (2.8) for the overlap integral and the factors $(-w_p)$ and $(1+w_p)$ are written out in terms of u, the overlap integral $\langle\eta_0,n_0|\,|\eta,n\rangle$ goes over into the form

$$\begin{aligned} &\langle\eta_0,n_0|\,|\eta,n\rangle \\ &\quad=(4\eta_0\eta)^{\gamma+1}\left[\frac{(n_0-1)!}{(n_0+2\gamma)!}\right]^{1/2}\left[\frac{(n+2\gamma)!}{(n-1)!}\right]^{1/2} \\ &\qquad\times\frac{1}{2\pi i}\oint_{(0+)} du\,\frac{(1+u)^{n_0+2\gamma}}{u^{n_0}} \\ &\qquad\times\frac{(\eta_0-\eta+2u\eta_0)^{n-1}}{(\eta_0+\eta+2u\eta_0)^{n+2\gamma+1}}\,. \end{aligned} \tag{2.13}$$

Notice that the final u integral is again of the Gaussian hypergeometric type. Accordingly one final linear transformation is all that is needed to evaluate the overlap integral. This time the transformation is chosen to map $u_p=-(\eta_0+\eta)/(2\eta_0)$ into the point at infinity, while leaving $u=0$ and $u=-1$ invariant. The factor $(\eta_0+\eta+2u\eta_0)^{n+2\gamma+1}$ is thereby eliminated from the integrand. The factor $(\eta_0-\eta+2u\eta_0)^{n-1}$ that remains is expanded by the binomial theorem, and the integral performed term by term using Eq. (2.12). The result is the expression (2.4) for the overlap integral. These final steps in the derivation need not be presented here in detail, since the results needed for the Green's function calculation of Sec. III are already in place: the representation (2.13) of the overlap integral forms the starting point for the Green's function calculation of Sec. III.

III. STURMIAN REPRESENTATION OF THE COULOMB GREEN'S FUNCTION

The discrete representation

$$\begin{aligned} &g=S\left[\frac{r}{2}\right]^{1/2}\sum_{nLJM}\frac{|\eta,nLJM\rangle\langle\eta,nLJM|}{(\gamma+n)\eta-EZ\alpha}\left[\frac{r}{2}\right]^{1/2}S^{-1}, \\ &S\equiv\cosh(\theta/2)+i\sigma\cdot\hat{r}\sinh(\theta/2)\,, \\ &\theta\equiv\tanh^{-1}(Z\alpha/K)\,,\quad K\equiv\sigma\cdot\mathbf{L}+1\,, \end{aligned} \tag{3.1}$$

of the Coulomb Green's function of the second-order Dirac equation has been derived earlier.[4] The derivation exploits the Coulomb Sturmian basis set (2.2), with $\eta\equiv(m^2-E^2)^{1/2}$. The energy is for the moment assumed to be a real number lying in the range $|E|<E_{\text{ground state}}$. This restriction can be lifted later by means of an analytic continuation argument.

As indicated in the Introduction, Coulomb Sturmian matrix elements will be investigated not for g itself, but for $r^{1/2}gr^{1/2}$. Accordingly, Eq. (3.1) is rewritten as

$$\begin{aligned} &r^{1/2}gr^{1/2}\equiv(rS)\mathbf{g}(rS^{-1}), \\ &\mathbf{g}=\frac{1}{2\eta}\sum_{nLJM}\frac{|\eta,nLJM\rangle\langle\eta,nLJM|}{(\gamma+n)-EZ\alpha/\eta}\,, \end{aligned} \tag{3.2}$$

and the matrix elements of rS, rS^{-1}, and $\mathbf{g}$ will be sought. The calculation of the matrix elements of rS and rS^{-1} is of a rather trivial nature, and is discussed in the Appendix. Here a closed expression for $\langle\eta_0,n_2,L,J,M\,|\mathbf{g}|\eta_0,n_1,L,J,M\rangle$, in terms of Gaussian hypergeometric functions, will be obtained. Note that, due to the diagonal nature of $\mathbf{g}$ in the angular momentum quantum numbers, the matrix elements $\langle\eta_0,n_2,L,J,M\,|\mathbf{g}|\eta_0,n_1,L,J,M\rangle$ are the only nonzero ones. The real parameter $\eta_0>0$ can be quite arbitrary. From Eq. (3.2) the desired matrix element can be written in terms of the radial parts of the Sturmian functions as

$$\begin{aligned} &\langle\eta_0 n_2 LJM\,|\mathbf{g}|\eta_0 n_1 LJM\rangle \\ &\quad=\sum_{n=1}^{\infty}\frac{1}{2\eta}\,\frac{\langle\eta_0 n_2 LJ|\,|\eta nLJ\rangle\langle\eta nLJ|\,|\eta_0 n_1 LJ\rangle}{\gamma+n-\kappa}\,, \\ &\quad\kappa\equiv EZ\alpha/\eta\,. \end{aligned} \tag{3.3}$$

Next, the overlap integrals in Eq. (3.3) are represented by contour integrals according to Eq. (2.13),

$$\langle \eta_0 n_2 LJM \,|\mathbf{g}|\, \eta_0 n_1 LJM \rangle$$

$$= \frac{(4\eta_0\eta)^{2\gamma+2}}{2\eta}\left[\frac{(n_2-1)!(2\gamma+1)!}{(n_2+2\gamma)!}\right]^{1/2}\left[\frac{(n_1-1)!(2\gamma+1)!}{(n_1+2\gamma)!}\right]^{1/2}\frac{1}{2\pi i}\oint du\,\frac{(1+u)^{n_2+2\gamma}}{u^{n_2}}\,\frac{1}{(\eta_0+\eta+2u\eta_0)^{2\gamma+2}}$$

$$\times\frac{1}{2\pi i}\oint dw\,\frac{(1+w)^{n_1+2\gamma}}{w^{n_1}}\,\frac{1}{(\eta_0+\eta+2w\eta_0)^{2\gamma+2}}\sum_{n=1}^{\infty}\frac{(n+2\gamma)!}{(n-1)!(2\gamma+1)!}\,\frac{\Xi^{n-1}}{\gamma+n-\kappa},$$

$$\Xi\equiv\frac{(\eta_0-\eta+2u\eta_0)(\eta_0-\eta+2w\eta_0)}{(\eta_0+\eta+2u\eta_0)(\eta_0+\eta+2w\eta_0)}. \tag{3.4}$$

The infinite series in Eq. (3.4) can be summed by means of the binomial expansion

$$(1-z)^{-\nu}=\sum_{n=0}^{\infty}\frac{(\nu-1+n)!}{(\nu-1)!n!}z^n,\quad |z|<1. \tag{3.5}$$

In order to achieve this, the identity $\int_0^1 dt\, t^{n+\gamma-1-\kappa}=1/(n+\gamma-\kappa)$ is employed to replace the denominator $1/(n+\gamma-\kappa)$ by a power. There is an assumption $n+\gamma-\kappa>0$ needed here to ensure convergence of the t integral. This convergence condition is obeyed under the restriction noted above that $|E|<E_{\text{ground state}}$. When these changes are incorporated the matrix element takes the form

$$\langle \eta_0 n_2 LJM \,|\mathbf{g}|\, \eta_0 n_1 LJM \rangle$$

$$= (2\eta)^{2\gamma+1}\left[\frac{(n_2-1)!(2\gamma+1)!}{(n_2+2\gamma)!}\right]^{1/2}\left[\frac{(n_1-1)!(2\gamma+1)!}{(n_1+2\gamma)!}\right]^{1/2}\int_0^1 dt\, t^{\gamma-\kappa}\frac{1}{2\pi i}\oint du\,\frac{(1+u)^{n_2+2\gamma}}{u^{n_2}}(\eta_0+\eta+2u\eta_0)^{-2\gamma-2}$$

$$\times\left[1-t\frac{\eta_0-\eta+2u\eta_0}{\eta_0+\eta+2u\eta_0}\right]^{-2\gamma-2}\frac{1}{2\pi i}\oint dw\frac{(1+w)^{n_1+2\gamma}}{w^{n_1}}(w-w_p)^{-2\gamma-2},$$

$$w_p\equiv-\frac{\eta_0+\eta}{2\eta_0}\left[1-t\left[\frac{\eta_0-\eta+2u\eta_0}{\eta_0+\eta+2u\eta_0}\right]\left[\frac{\eta_0-\eta}{\eta_0+\eta}\right]\right]\left[1-t\left[\frac{\eta_0-\eta+2u\eta_0}{\eta_0+\eta+2u\eta_0}\right]\right]^{-1}. \tag{3.6}$$

The w integral encountered in Eq. (3.6) is of the Gaussian hypergeometric type, and is in fact identical to the integral (2.11) already evaluated, aside from the different meaning of w_p. Using Eq. (2.11), and writing out all terms involving w_p in terms of u, gives

$$\langle \eta_0 n_2 LJM \,|\mathbf{g}|\, \eta_0 n_1 LJM \rangle = (-1)^{n_1-1}\frac{(4\eta\eta_0)^{2\gamma+2}}{2\eta}\left[\frac{(n_2-1)!}{(n_2+2\gamma)!}\right]^{1/2}\left[\frac{(n_1+2\gamma)!}{(n_1-1)!}\right]^{1/2}\int_0^1 dt\, t^{\gamma-\kappa}\frac{1}{2\pi i}\oint du\frac{(1+u)^{n_2+2\gamma}}{u^{n_2}}$$

$$\times\frac{[(\eta_0+\eta+2u\eta_0)(\eta_0-\eta)-(\eta_0-\eta+2u\eta_0)(\eta_0+\eta)t\,]^{n_1-1}}{[(\eta_0+\eta+2u\eta_0)(\eta_0+\eta)-(\eta_0-\eta+2u\eta_0)(\eta_0-\eta)t\,]^{n_1+2\gamma+1}}. \tag{3.7}$$

The u integral in Eq. (3.7) is again of the hypergeometric type. The evaluation of the u integral begins with the linear transformation

$$u=\frac{su_p}{s+1+u_p},\quad u_p\equiv-\frac{1}{\zeta}\frac{1-t(1-\zeta)^2}{1+t(1+\zeta)},\quad \zeta\equiv\frac{2\eta_0}{\eta_0+\eta}, \tag{3.8}$$

which has the effect of eliminating the factor

$$[(\eta_0+\eta+2u\eta_0)(\eta_0+\eta)-(\eta_0-\eta+2u\eta_0)(\eta_0-\eta)t\,]^{-(n_1+2\gamma+1)}$$

from the integrand, while preserving the general structure

$$u^{-n_2}(1+u)^{n_2+2\gamma}.$$

The result of the linear transformation to the complex s plane is

$$\langle \eta_0 n_2 LJM \,|\mathbf{g}|\, \eta_0 n_1 LJM \rangle$$

$$=\frac{1}{2\eta_0}\zeta^{2\gamma+3}(2-\zeta)^{2\gamma+1}(1-\zeta)^{n_2-n_1}\left[\frac{(n_2-1)!}{(n_2+2\gamma)!}\right]^{1/2}\left[\frac{(n_1+2\gamma)!}{(n_1-1)!}\right]^{1/2}\int_0^1 dt\, t^{\gamma-\kappa}\frac{(1-t)^{n_2-n_1}}{(1-t(1-\zeta)^2)^{n_2+n_1+2\gamma}}$$

$$\times\frac{1}{2\pi i}\oint ds\,\frac{1+s)^{n_2+2\gamma}}{s^{n_2}}[(1-\zeta)^2(1-t)^2+ts\zeta^2(2-\zeta)^2]^{n_1-1}. \tag{3.9}$$

The result of the s integration is a hypergeometric function that breaks off to form a polynomial of order $\min(n_2 n_1)$:

$$\langle \eta_0 n_2 LJM\,|\mathbf{g}|\,\eta_0 n_1 LJM\rangle$$
$$= \frac{1}{2\eta_0}\xi^{2\gamma+3}(2-\xi)^{2\gamma+1}(1-\xi)^{n_2-1+n_1-1}\frac{1}{(2\gamma+1)!}\left[\frac{(n_2+2\gamma)!}{(n_2-1)!}\right]^{1/2}\left[\frac{(n_1+2\gamma)!}{(n_1-1)!}\right]^{1/2}$$
$$\times\int_0^1 dt\, t^{\gamma-\kappa}\frac{(1-t)^{n_2-1+n_1-1}}{(1-t(1-\xi)^2)^{n_2+n_1+2\gamma}}\,{}_2F_1(-(n_2-1),-(n_1-1),2\gamma+2;\Lambda)\,,\quad \Lambda\equiv\frac{t}{(1-t)^2}\frac{\xi^2(2-\xi)^2}{(1-\xi)^2}\,. \tag{3.10}$$

It is now an easy step to complete the calculation and obtain a closed expression for the matrix element. The hypergeometric polynomial ${}_2F_1(-(n_2-1),-(n_1-1),2\gamma+2;\Lambda)$ is expanded in a series, and the integral over t is performed term by term, with the result

$$\langle \eta_0 n_2 LJM\,|\mathbf{g}|\,\eta_0 n_1 LJM\rangle$$
$$= \frac{1}{2\eta_0}\xi^{2\gamma+3}(2-\xi)^{2\gamma+1}(1-\xi)^{n_2-1+n_1-1}\frac{1}{(2\gamma+1)!}\left[\frac{(n_2+2\gamma)!}{(n_2-1)!}\right]^{1/2}\left[\frac{(n_1+2\gamma)!}{(n_1-1)!}\right]^{1/2}$$
$$\times\sum_{p=0}^{n_<-1}\frac{(-(n_2-1))_p(-(n_1-1))_p}{(2\gamma+2)_p}\frac{[\xi^2(2-\xi)^2/(1-\xi)^2]^p}{p!}\frac{\Gamma(\gamma+p+1-\kappa)(n_1+n_2-2-2p)!}{\Gamma(\gamma+n_1+n_2-p-\kappa)}$$
$$\times{}_2F_1(n_1+n_2+2\gamma,\gamma+p+1-\kappa,\gamma+n_1+n_2-p-\kappa;(1-\xi)^2)\,. \tag{3.11}$$

The result (3.11) has been confirmed by an independent calculation in which the matrix elements are derived from the coordinate space representation of the Coulomb Green's function,[23] and using integral representations from the theory of special functions.[24]

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APPENDIX: MATRIX ELEMENTS OF THE FACTORS rS AND rS^{-1}

Matrix elements of the operators

$$rS = r\cosh(\theta/2) + ri\sigma\cdot\hat{r}\sinh(\theta/2) \tag{A1}$$

and

$$rS^{-1} = r\cosh(\theta/2) - ri\sigma\cdot\hat{r}\sinh(\theta/2)\,,\quad \theta\equiv\tanh^{-1}(Z\alpha/K),\ K=\sigma\cdot\mathbf{L}+1, \tag{A2}$$

will be considered briefly. The fact that θ is diagonal in the angular momentum quantum numbers L, J, M makes the calculation relatively easy: $\langle \eta_0,n_2,L,J,M\,|r|\eta_0,n_1,L,J,M\rangle$ is the key matrix element needed for the $\cosh(\theta/2)$ terms of rS and rS^{-1}. The result

$$\langle \eta_0 n_2 LJM\,|2\eta_0 r|\eta_0 n_1 LJM\rangle$$
$$= 2(\gamma+n_2)\delta_{n_2,n_1} - (n_2(n_2+1+2\gamma))^{1/2}\delta_{n_2+1,n_1} - ((n_2-1)(n_2+2\gamma))^{1/2}\delta_{n_2-1,n_1} \tag{A3}$$

for this matrix element incorporates the identities[25]

$$xL_n^{\mu}(x) = (\mu+1+2n)L_n^{\mu}(x) - (n+\mu)L_{n-1}^{\mu}(x) - (n+1)L_{n+1}^{\mu}(x) \tag{A4}$$

and[26]

$$\int_0^{\infty} dx\, x^{\mu}e^{-x}L_n^{\mu}(x)L_m^{\mu}(x) = \frac{(n+\mu)!}{n!}\delta_{n,m}\,. \tag{A5}$$

Similar results can be obtained for the terms of rS and rS^{-1} involving $\sinh(\theta/2)$. This time the operator is diagonal in J and M, but not in L. The identity $\sigma\cdot\hat{r}Y_{LJM}(\hat{r}) = Y_{L'JM}(\hat{r})$, where $L+L'=2J$, provides selection rules according to which the key nonzero matrix elements needed are now of the type

$$\langle \eta_0,n_2,J-\tfrac{1}{2},JM\,|2\eta_0 r|\eta_0,n_1,J+\tfrac{1}{2},JM\rangle,$$

or

$$\langle \eta_0,n_2,J+\tfrac{1}{2},JM\,|2\eta_0 r|\eta_0,n_1,J-\tfrac{1}{2},JM\rangle.$$

The equation

$$\langle \eta_0,n_2,L_2=J-\tfrac{1}{2},JM\,|2\eta_0 r|\eta_0,n_1,L_1=J+\tfrac{1}{2},JM\rangle$$
$$= \delta_{n_2,n_1}[(n_1+2\gamma_1)(n_1+2\gamma_1-1)]^{1/2} - 2\delta_{n_2,n_1+1}[n_1(n_1+2\gamma_1)]^{1/2} + \delta_{n_2,n_1+2}[n_1(n_1+1)]^{1/2} \tag{A6}$$

and the analogous equation for

$$\langle \eta_0,n_2,J+\tfrac{1}{2},JM\,|2\eta_0 r|\eta_0,n_1,J-\tfrac{1}{2},JM\rangle$$

can be obtained using the identity[27]

$$L_{n-1}^{2\gamma-1}(x) = L_{n-1}^{2\gamma+1}(x) - 2L_{n-2}^{2\gamma+1}(x) + L_{n-3}^{2\gamma+1}(x), \tag{A7}$$

and Eq. (A5).

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[25]See Ref. 21. p. 137, Eq. (10b).
[26]See Ref. 21, p. 136, Eq. (9).
[27]See Ref. 21, p. 137, Eq. (10g) implies the relationship $nL_n^\mu(x) - (\mu+n)L_{n-1}^\mu(x) = -\mu L_n^\mu(x) + (\mu+n)L_n^{\mu-1}(x)$, or $L_n^\mu(x) - L_{n-1}^\mu(x) = L_n^{\mu-1}(x)$. This last identity used two times leads to Eq. (A7) in the Appendix.

A note on the electron self-energy

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Using dimensional regularization, the lowest-order electron self-energy function in an arbitrary covariant gauge is derived. For off-mass-shell electrons, the usual expression for the finite portion Σ_f of the self-energy as the number of space-time dimensions n approaches 4 is recovered. In the case of on-mass-shell electrons, the condition $(\not p - m)\Sigma_f \to 0$ as $\not p \to m$, which is necessary to make the usual separation of the renormalization constant unambiguous, requires that n approach 4 from above, i.e., $n \to 4_+$. This necessary condition on Σ_f is not satisfied by the off-mass-shell expression in the limit $p^2 \to m^2$ due to a branch point in the self-energy operator.

I. INTRODUCTION

The separation of renormalization constants from finite quantities in renormalizable field theories is a time-honored process which is facilitated by the use of regularization techniques.[1-3] In quantum electrodynamics, the necessity for a regularization scheme to respect gauge invariance was emphasized by Gupta.[2] Consistency with gauge invariance together with ease of implementation makes the dimensional regularization technique[3] a particularly attractive alternative to regulator schemes involving covariant cutoffs. While applying dimensional regularization for certain radiative corrections to positronium energy levels and decays,[4] we encountered a question, which may be of general interest, about how the renormalization constant associated with the electron self-energy $\Sigma(p)$ is separated from the finite part.

Recall that regardless of the method one may use for regularization, it is convenient to express the regularized $\Sigma(p)$ as

$$\Sigma(p) = A + (\not p - m)B + (\not p - m)^2\Sigma_f(p), \tag{1}$$

where A and B are independent of the electron four-momentum p, and

$$(\not p - m)\Sigma_f(p)\big|_{\not p \to m} = 0, \tag{2}$$

in order to have a unique decomposition in Eq. (1).

Evaluation of A is straightforward, whereas for B and Σ_f, some care must be exercised.[5] We should mention that the Σ_f, which is usually found in literature,[6] does not satisfy the condition given in Eq. (2).

In this paper we calculate the $\Sigma(p)$ in an arbitrary covariant gauge using dimensional regularization and express it in the form of Eq. (1). Assuming that the electron is off-mass-shell, we recover the usual expression for Σ_f as the number of dimensions $n \to 4$. For an on-mass-shell electron, our general expression for Σ_f satisfies Eq. (2) if we assume that the dimension of space-time is larger than 4 ($n \to 4_+$).

Throughout our paper, we use the notation and conventions of Bjorken and Drell.[7] We also use the natural units $\hbar = c = 1$.

II. ELECTRON SELF-ENERGY

Using dimensional regularization, the lowest-order electron self-energy in an arbitrary covariant gauge can be written as[8]

$$\Sigma(p) = -ie^2 \int \frac{d^n k}{(2\pi)^4} \gamma^\mu \frac{1}{\not p - \not k - m + i\eta} \times \gamma^\nu \frac{1}{k^2}\left(g_{\mu\nu} + \epsilon \frac{k_\mu k_\nu}{k^2}\right). \tag{3}$$

Employing Feynman parametrization and performing the integrals on k, we find

$$\Sigma(p) = (\alpha/4\pi)\Gamma(-a) I_1(p) - (\alpha\epsilon/4\pi) m^{-2}\Gamma(1-a) I_2(p), \tag{4}$$

where

$$I_1(p) = \sum_{\beta=0}^{2} g_\beta(p)\rho^a \int_0^1 dx\, x^{a+\beta}\left(1 - \frac{\rho - 1}{\rho} x\right)^a,$$
$$I_2(p) = \sum_{\beta=0}^{2} h_\beta(p)\rho^{a-1} \times \int_0^1 dx\, x^{a+\beta+1}\left(1 - \frac{\rho-1}{\rho} x\right)^{a-1}, \tag{5}$$

with

$$\rho = (-p^2 + m^2)/m^2 - i\eta \quad (\eta > 0),$$
$$a = n/2 - 2 \quad (a \neq 0,1,2,\ldots), \tag{6}$$

and we disregarded any overall multiplicative constant of the form C^a. The coefficients g_β and h_β are

$$g_0(p) = -(2 + \epsilon + 2a + \epsilon a)\not p + (4 + 2\epsilon + 2a + \epsilon a)m,$$
$$g_1(p) = (2 - 2\epsilon + 2a)\not p - (2\epsilon + \epsilon a)m, \tag{7}$$
$$g_2(p) = (3\epsilon + \epsilon a)\not p,$$

and

$$h_0(p) = p^2 \not p + p^2 m,$$
$$h_1(p) = -2p^2 \not p - p^2 m, \tag{8}$$
$$h_2(p) = p^2 \not p.$$

The integrals in I_1 and I_2 can be performed and expressed in terms of hypergeometric functions (Ref. 9, Eq. 3.194 1),

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$$I_1(p)=\sum_{\beta=0}^{2} g_\beta(p)\frac{\rho^a}{a+\beta+1}\times F\left(-a,a+\beta+1;a+\beta+2;\frac{\rho-1}{\rho}\right),$$
$$I_2(p)=\sum_{\beta=0}^{2} h_\beta(p)\frac{\rho^{a-1}}{a+\beta+2}\times F\left(-a+1,a+\beta+2;a+\beta+3;\frac{\rho-1}{\rho}\right), \tag{9}$$

with $a\neq -2,-3,\ldots$, and we have used the notation $F\equiv {}_2F_1$.

By using the analytic continuation of hypergeometric functions for the region $|\rho|<1$, and expanding them in terms of a (see the Appendix), we obtain

$$I_1(p)=\sum_{\beta=0}^{2} g_\beta(p)\lambda_\beta(\rho)\,,\qquad I_2(p)=\sum_{\beta=0}^{2} h_\beta(p)\Lambda_\beta(\rho)\,, \tag{10}$$

where, for $0<|a|<\frac{1}{2}$ and $|\rho|<1$,

$$\lambda_0(\rho)=1-2a+(\rho^{2a}-1)[\rho/2(1-\rho)]\times\{-1+[2+\ln(1-\rho)]a\}+O(a^2)\,,$$
$$\lambda_1(\rho)=\frac{1}{2}+\frac{2\rho-1}{2(1-\rho)}a+(\rho^{2a}-1)\frac{\rho^2}{4(1-\rho)^2}\times\{1+[-2-\ln(1-\rho)]a\}+O(a^2)\,, \tag{11}$$
$$\lambda_2(\rho)=\frac{1}{3}+\frac{-13\rho^2+11\rho-4}{18(1-\rho)^2}a+(\rho^{2a}-1)\frac{\rho^3}{6(1-\rho)^3}\times\left\{-1+\left[\frac{13}{6}+\ln(1-\rho)\right]a\right\}+O(a^2)\,,$$

and

$$\Lambda_0(\rho)=\frac{1}{1-\rho}+(\rho^{2a}-1)\frac{\rho}{2(1-\rho)^2}\times\left[\frac{1}{a}-1-\ln(1-\rho)\right]+O(a)\,,$$
$$\Lambda_1(\rho)=\frac{1-3\rho}{2(1-\rho)^2}+(\rho^{2a}-1)\frac{\rho^2}{2(1-\rho)^3}\times\left[-\frac{1}{a}+\frac{3}{2}+\ln(1-\rho)\right]+O(a)\,, \tag{12}$$
$$\Lambda_2(\rho)=\frac{11\rho^2-7\rho+2}{6(1-\rho)^3}+(\rho^{2a}-1)\frac{\rho^3}{2(1-\rho)^4}\times\left[\frac{1}{a}-\frac{11}{6}-\ln(1-\rho)\right]+O(a)\,.$$

By inserting these expansions into Eq. (4) and rearranging terms, we find

$$\Sigma(p)=\frac{\alpha m}{4\pi}\Gamma(-a)(3-4a)+\frac{\alpha}{4\pi}\Gamma(-a)(\not p-m)\times\left[-1-\epsilon+\left(2+\frac{5}{3}\epsilon\right)a\right]+\frac{\alpha}{4\pi}\Gamma(1-a)\times(\not p-m)\left(\frac{2-\epsilon}{a}-2+\frac{5}{3}\epsilon\right)+\tilde\Sigma(p)\,, \tag{13}$$

where

$$\tilde\Sigma(p)=\frac{\alpha}{4\pi}\left[(\not p-m)\left(\frac{\epsilon-2}{a}+2-2\epsilon\right)-\frac{(\epsilon+1)\rho\not p}{1-\rho}\right]\times\Gamma(1-a)+\frac{\alpha}{4\pi}(\rho^{2a}-1)\frac{\rho}{2(1-\rho)}\times\left\{-(2+\epsilon)m+\left[\frac{(1+\epsilon)(2-\rho)\not p}{1-\rho}-(4+\epsilon)m\right]\left[-\frac{1}{a}+1+\ln(1-\rho)\right]\right\}\times\Gamma(1-a). \tag{14}$$

The term $1/a$ reflects the infrared divergence, while the factor $(\not p-m)$ in the second term of Eq. (13) comes from $(\not p-m)$ dependence of $g_\beta(p)$, and its coefficient gives the ultraviolet divergence.

We write Eq. (13) in the following compact form:

$$\Sigma(p)=A+(\not p-m)B+(\not p-m)^2\Sigma_f(p), \tag{15}$$

where

$$A=(\alpha m/4\pi)\Gamma(-a)(3-4a)\,, \tag{16}$$

is the (gauge independent) self-mass,

$$B=\frac{\alpha}{4\pi}\Gamma(-a)(-1-\epsilon+4a)+\frac{\alpha}{4\pi}\Gamma(1-a)\frac{2-\epsilon}{a}\,, \tag{17}$$

is related to the wave function renormalization constant, and we have used the following definition:

$$\tilde\Sigma(p)=(\not p-m)^2\Sigma_f(p)\,. \tag{18}$$

Using the identities

$$(\not p-m)=[-(\not p+m)/m^2\rho](\not p-m)^2,\qquad 1=[(2\not p-m\rho+2m)/m^3\rho^2](\not p-m)^2\,, \tag{19}$$

and Eqs. (14) and (18), we find

$$\Sigma_f(p)=\frac{\alpha}{4\pi m}\Gamma(1-a)\left\{\frac{1+\epsilon}{1-\rho}+(2+\epsilon)C+(\epsilon-2+3\rho)D-\frac{\not p+m}{m\rho}\left[\frac{\epsilon-2}{a}+\frac{4+(\epsilon-3)\rho}{1-\rho}+(4+2\epsilon)C+(2\epsilon-4+(4-2\epsilon)\rho+(1+\epsilon)\rho^2)D\right]\right\}, \tag{20}$$

where

$$C=(\rho^{2a}-1)/2(1-\rho)\,, \tag{21}$$
$$D=[(\rho^{2a}-1)/2(1-\rho)^2][1/a-1-\ln(1-\rho)]\,. \tag{22}$$

Henceforth, we restrict the values of a to $0<a<\frac{1}{2}$ [this is a necessary condition in order to satisfy Eq. (2), see Eq. (25)].

The expression for $\Sigma_f(p)$ can be simplified (in terms of a) if we write it in two separate forms, one for $\rho = 0$, and the other for $0 < |\rho| < 1$. In the following we use the notation

$$\Sigma_f(p)\,|_{\not p = m} \equiv \Sigma_f^{\rm on}\,, \tag{23}$$

$$\Sigma_f(p)\,|_{\not p \neq m} \equiv \Sigma_f^{\rm off}\,. \tag{24}$$

For $\rho = 0$ ($\not p = m$), we have $\lim_{\rho\to 0}\rho^{2a}\to 0$, and find

$$\Sigma_f^{\rm on} = \frac{\alpha}{4\pi m}[\,(-3+\tfrac{3}{2}\epsilon)/a + (1+\epsilon) - \rho^{2a-1}((2\epsilon-4)/a+8)]\Gamma(1-a)\,. \tag{25}$$

For $0<|\rho|<1$ ($\not p \neq m$), we use the expansion $\rho^{2a} = 1 + 2a\ln\rho$, and find

$$\Sigma_f^{\rm off}(p) = \frac{\alpha}{4\pi m}\left\{\frac{1+\epsilon}{1-\rho} + \frac{3\rho+\epsilon-2}{(1-\rho)^2}\ln\rho - \frac{\not p + m}{m\rho}\left[\frac{(\epsilon-3)\rho+4}{1-\rho} + \frac{(1+\epsilon)\rho^2+(4-2\epsilon)\rho+(2\epsilon-4)}{(1-\rho)^2}\ln\rho + \frac{\epsilon-2}{a}\right]\right\}\Gamma(1-a)\,. \tag{26}$$

Notice that $\lim_{\not p\to m}(\not p - m)\Sigma_f^{\rm on}(p)\to 0$ (this is not true for $\Sigma_f^{\rm off}$). This relation assures that our decomposition of $\Sigma(p)$ in Eq. (15) is unique. It also guarantees that after mass renormalization, the electron propagator (near-mass-shell) will be modified, due to the self-energy correction, by a multiplicative factor. We can extend the domain of $\Sigma_f^{\rm off}$ by analytic continuation. It will have the same form for $|\rho|\geqslant 1$.

If we are not interested in a single expression for $\Sigma_f(p)$ for whole region $|\rho|<1$, we can find $\Sigma_f^{\rm on}$ by keeping only those terms in expansions of hypergeometric functions [see Eq. (A3)] which are up to the second order in ρ. For $\Sigma_f^{\rm off}$, it is much easier to use the original Eq. (9), which can be expanded in terms of ρ in region $\mathrm{Re}(\rho) > \frac{1}{2}$, and by analytic continuation it can be shown that it has the same form for all ρ (except at $\rho = 0$).

III. SUMMARY AND CONCLUSIONS

Our main objective for representing $\Sigma_f(p)$ by a single expression is to show, in a clear way, that the inequality $\lim_{\not p\to m}\Sigma_f^{\rm off}(p) \neq \Sigma_f^{\rm on}$ is due to the use of the expansion $\rho^{2a} = 1 + 2a\ln\rho$ in finding $\Sigma_f^{\rm off}$, which is justified only for $\rho\neq 0$.

For one-loop corrections, the difference between $\Sigma_f^{\rm on}$ and $\lim_{\not p\to m}\Sigma_f^{\rm off}$ does not present a problem since ρ is a nonvanishing constant in these cases. However, when dealing with multiloop corrections, some thought must be given to the values of the integration variable encountered in expressions containing Σ_f. In such circumstances, it is entirely possible that the surface $\rho = 0$ could make a significant contribution which is sensitive to the difference between $\Sigma_f^{\rm on}$ and $\lim_{\not p\to m}\Sigma_f^{\rm off}$. If this is the case, then one should employ Eq. (20) for $\Sigma_f(p)$, which is correct for all values of p.

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APPENDIX: REDUCTION OF $I_1(\rho)$ AND $I_2(\rho)$

The analytic continuation of $F(a,b;b+1;(\rho-1)/\rho)$ to the region $|\rho|<1$ can be found by the relation[10]

$$F\left(a,b;b+1;\frac{\rho-1}{\rho}\right) = \frac{b\rho^a}{b-a}F(a,1;a-b+1;\rho) + \frac{\Gamma(b+1)\Gamma(a-b)}{\Gamma(a)}\left(\frac{\rho}{1-\rho}\right)^b, \tag{A1}$$

with condition $|\arg(1/\rho)|<\pi$, which can be satisfied [even for real values of four-momentum p, since $\rho = (-p^2 + m^2)/m^2 - i\eta$, $\eta>0$].

In this Appendix we work out $F(-a+1,a+2;a+3;(\rho-1)/\rho)$; the other F's can be found in a similar way.

From Eq. (A1) we obtain

$$F\left(1-a,a+2;a+3;\frac{\rho-1}{\rho}\right) = \frac{(a+2)\rho^{1-a}}{2a+1}F(1-a,1;-2a;\rho) + \frac{\Gamma(a+3)\Gamma(-1-2a)}{\Gamma(1-a)}\left(\frac{\rho}{1-\rho}\right)^{a+2}. \tag{A2}$$

Using the formula

$$F(a,1;c;\rho) = \frac{\Gamma(c)}{\Gamma(a)}\sum_{m=0}^{\infty}\frac{\Gamma(a+m)}{\Gamma(c+m)}\rho^m\,,\quad |\rho|<1\,, \tag{A3}$$

we find

$$F(-a+1,1;-2a;\rho) = 1 + \frac{1}{-2a}\frac{\Gamma(-2a+1)}{\Gamma(-a+1)} \times \sum_{m=1}^{\infty}\frac{\Gamma(-a+1+m)}{\Gamma(-2a+m)}\rho^m\,. \tag{A4}$$

Notice that in the closed region of an annular ring which is bounded by two concentric circles centered at origin of the a plane, with radii ϵ_1 and $\frac{1}{2}-\epsilon_2$ (ϵ_1 and ϵ_2 are positive but much smaller than 1), $\Gamma(-2a+1)/\Gamma(-a+1)$ and $\Gamma(-a+1+m)/\Gamma(-2a+m)$ are analytic functions of a, and the series in Eq. (A4) is uniformly convergent ($|\rho|<1$) and consequently its sum is an analytic function of a. Therefore $F(-a+1,1;-2a;\rho)$ itself is an analytic function of a and we can expand it about $a = 0$,

$$F(-a+1,1;-2a;\rho)$$
$$=1+\frac{1}{-2a}\left\{\sum_{m=1}^{\infty} m\rho^m + a\sum_{m=1}^{\infty}\frac{\partial}{\partial a}\left[\frac{\Gamma(-2a+1)}{\Gamma(-a+1)}\times\frac{\Gamma(-a+1+m)}{\Gamma(-2a+m)}\right]_{a=0}\rho^m + O(a^2)\right\}$$
$$=\frac{2-3\rho}{2(1-\rho)^2}+\frac{\rho}{2(1-\rho)^2}\ln(1-\rho)$$
$$+\frac{-\rho}{2(1-\rho)^2}\frac{1}{a}+O(a)\,. \tag{A5}$$

In derivation of Eq. (A5) we have used the following formulas (Ref. 9. Eqs. 8.36 and 1.513 6):

$$\frac{\Gamma'(m+1)}{\Gamma(m+1)}-\frac{\Gamma'(1)}{\Gamma(1)}=\sum_{k=1}^{m}\frac{1}{k}\,,\quad m=1,2,3,\ldots\,, \tag{A6}$$

$$\sum_{m=1}^{\infty}\left(\sum_{k=1}^{m}\frac{1}{k}\right)\rho^m=\frac{-1}{1-\rho}\ln(1-\rho)\,, \tag{A7}$$

$$\sum_{m=0}^{\infty}\rho^m=\frac{1}{1-\rho}\,. \tag{A8}$$

with their derivatives with respect to ρ (after multiplying by appropriate powers of ρ).

For the second term of $F(-a+1,a+2;a+3;(\rho-1)/\rho)$ in Eq. (A2), we obtain

$$\frac{\Gamma(a+3)\Gamma(-2a-1)}{\Gamma(-a+1)}\left(\frac{\rho}{1-\rho}\right)^{a+2}$$
$$=\frac{1}{(-2a-1)(-2a)}\frac{\Gamma(a+3)\Gamma(-2a+1)}{\Gamma(-a+1)}$$
$$\times\frac{\rho^{a+2}}{(1-\rho)^2}[1-a\ln(1-\rho)+O(a^2)]$$
$$=\frac{\rho^{a+2}}{(1-\rho)^2}\left[\frac{1}{a}-\frac{1}{2}-\ln(1-\rho)\right]+O(a)\,, \tag{A9}$$

where we have used the expansion

$$(1-\rho)^{-a}=1-a\ln(1-\rho)+O(a^2),\quad |\rho|<1\,. \tag{A10}$$

Therefore, combining (A2), (A5), and (A9), we find, for $|\rho|<1$,

$$F\left(-a+1,a+2;a+3;\frac{\rho-1}{\rho}\right)$$
$$=\frac{\rho^{a+2}}{(1-\rho)^2}\left[\frac{1}{a}-\frac{1}{2}-\ln(1-\rho)\right]+\frac{\rho^{2-a}}{(1-\rho)^2}$$
$$\times\left[-\frac{1}{a}-\frac{3}{2}+\frac{2}{\rho}+\ln(1-\rho)\right]+O(a)\,. \tag{A11}$$

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Chiral symmetry breakdown. III. Delbourgo's gauge technique

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The quark propagator in massless quantum chromodynamics (QCD) is analyzed using the gauge technique. In both the Feynman and Landau gauges with a Pauli–Villars cutoff, a chirally symmetric solution is found, while a nonsymmetric solution appears at a critical coupling $\lambda_c > 0$. As the cutoff is removed, λ_c tends to 0 but the nonsymmetric solution vanishes in the continuum limit, so that chiral symmetry is then restored.

I. INTRODUCTION

Spontaneous dynamical breakdown of chiral symmetry represents an interesting and potentially important means through which particles become massive at a certain critical coupling strength because of interactions with the quantum field.[1] In QCD, this phenomenon provides a mechanism for quarks to acquire constituent masses in a formally massless theory through nonperturbative effects. The occurrence of dynamical symmetry breaking is investigated by analysis of Dyson–Schwinger equations for the fermion propagator. Such analyses are hampered by a degree of arbitrariness, in that the effect of unavoidable truncation of Dyson–Schwinger equations is difficult to assess.

Some time ago Maskawa and Nakajima showed that, in the context of quantum electrodynamics (QED), when the fermion–fermion–photon vertex function and the photon propagator are replaced by their free values, the solutions of the Dyson–Schwinger equation exhibit spontaneous chiral symmetry breaking.[2] In a recent paper we demonstrated that this spontaneous symmetry breaking occurs when one introduces both an infrared and an ultraviolet cutoff.[3] In a more detailed analysis of the problem, this truncation procedure was found to be unacceptably gauge dependent. We showed that chiral symmetry was indeed broken in the theory with cutoffs present, but that the symmetry was restored in the continuum limit in certain gauges.[4] It was found that chiral symmetry breaking was very sensitive to the infrared and ultraviolet behavior of the gauge-dependent free photon propagator. Furthermore, we showed that this sensitivity to choice of gauge remained even when the truncation procedure was modified to maintain consistency with the "transversality" constraint coming from gauge invariance in the ultraviolet.[5] It is our conclusion that the free vertex approximation cannot provide a reliable indication as to the occurrence of spontaneous chiral symmetry breaking, and that other truncation schemes should be explored.

Truncation of Dyson–Schwinger equations is certainly an *ad hoc* procedure based primarily upon expediency, but one must make use of physically motivated conditions or requirements whenever possible. Several authors have chosen the quark–quark–gluon vertex in QCD to decrease as $1/\log q^2$ at large q^2, in correspondence with the ultraviolet behavior imposed by asymptotic freedom.[6–8] We have shown in Ref. 4 that chiral symmetry remains unbroken in certain gauges in the continuum limit in this case as well, because of formal divergence of the loop integral in the Dyson–Schwinger equation. We conclude that this truncation scheme has essentially the same difficulties as the free vertex approximation, and thus that one must look further to obtain a resolution of the ambiguity associated with gauge-dependent results.

The free vertex truncation, as well as its renormalization-group-improved counterpart discussed in Ref. 4, is not consistent with the Slavnov–Taylor identity, and therefore stands in direct conflict with the requirements of gauge invariance. The gauge dependence of the results on chiral symmetry breaking is a manifestation of the gauge dependence of the truncation scheme. By contrast, in the truncation scheme proposed some time ago by Salam and Delbourgo,[9] and studied by a number of people,[10,11] one maintains consistency with the Slavnov–Taylor identity for the vertex function, and thus the effects of gauge dependence should be reduced.

Here we will study chiral symmetry breaking in the Salam–Delbourgo scheme, which is based upon spectral *Ansätze* for the propagator and vertex functions. We replace the gluon propagator by a free massive one, and discuss both Feynmann and Landau gauges in the Dyson–Schwinger equation in Sec. II. The formal divergence of the loop integral is removed by introducing a Pauli–Villars cutoff; and the Dyson–Schwinger equation reduces to a homogeneous linear equation for the spectral density function, which has nontrivial solutions.

We find that when the cutoff is present, only a chirally symmetric solution occurs below a critical coupling $\lambda_c > 0$, whereas above λ_c nonsymmetric solutions are also present. In the continuum limit as the cutoff is removed, λ_c goes formally to 0. However, in both gauges only the chirally symmetric solution survives. Therefore in the Salam–Delbourgo formalism chiral symmetry is restored in the continuum limit.

II. SALAM–DELBOURGO ANSATZ

The Dyson–Schwinger equation for the quark propagator $S'_F(p)$ can be written

$$\not{p} S'_F(p) - \Sigma(p) S'_F(p) = 1, \tag{2.1}$$

where the self-energy is given by

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$$\Sigma(p) = \frac{ig^2}{(2\pi)^4} \int d^4k\, \gamma_\mu S'_F(p-k)\Gamma_\nu(p-k,p)D'^{\mu\nu}_F(k), \tag{2.2}$$

where Γ_ν is the gluon-quark vertex function and D'_F the gluon propagator. Here g is proportional to the SU(3) coupling constant.

The Lehmann representation for the quark propagator can be written

$$S'_F(p) = \int_{-\infty}^{\infty} dw' \frac{\rho(w')}{\not p - w' + i\epsilon\epsilon(w')}, \tag{2.3}$$

where $\epsilon(w') = \mathrm{sgn}(w')$, and ρ is an unknown spectral function. If $\rho(w)$ is even in w, $S'_F(p)$ has the form $\not p$ times a function of p^2, and so chiral symmetry is then unbroken. The Salam–Delbourgo *Ansatz* assumes that

$$S'_F(p-k)\Gamma_\nu(p-k,p)S'_F(p) = \int_{-\infty}^{\infty} dw'\rho(w') \frac{1}{\not p - \not k - w'} \gamma_\nu \frac{1}{\not p - w'}, \tag{2.4}$$

where the $i\epsilon\epsilon(w')$ is to be understood in both denominators. It is easy to see that (2.4) is consistent with the Slavnov–Taylor identity for Γ_ν.

With this *Ansatz*, the Dyson–Schwinger equation (2.1) can be rewritten in the form

$$\int_{-\infty}^{\infty} dw'\, \rho(w')[\not p - \Sigma(\not p - w')]\frac{1}{\not p - w'} = 1, \tag{2.5}$$

where

$$\Sigma(\not p, w') = \frac{ig^2}{(2\pi)^4} \int d^4k\, \gamma_\nu \frac{1}{\not p - \not k - w'} \gamma_\nu D'^{\mu\nu}_F(k). \tag{2.6}$$

In this paper, we propose to consider the Feynman and the Landau gauges. Moreover, we shall remove the divergence of the loop integral (2.6) by introducing a Pauli–Villars cutoff. We write

$$D'^{\mu\nu}_F(k) = D^{\mu\nu}(k,m) - D^{\mu\nu}(k,\Lambda), \tag{2.7}$$

where the cutoff Λ is much greater than m, the gluon mass, and where, in the Feynman gauge,

$$D^{\mu\nu}(k,m) = -g^{\mu\nu}/(k^2 - m^2 + i\epsilon), \tag{2.8a}$$

and in the Landau gauge,

$$D^{\mu\nu}(k,m) = \left[-g^{\mu\nu} + \frac{k^\mu k^\nu}{k^2 + i\epsilon}\right]\frac{1}{k^2 - m^2 + i\epsilon}. \tag{2.8b}$$

The corresponding expressions for Σ can be calculated:

$$\Sigma(\not p, w') = \lambda \int_{-\infty}^{\infty} dw \frac{\Omega(w,w',m) - \Omega(w,w',\Lambda)}{\not p - w}. \tag{2.9}$$

Here $\lambda = g^2/(16\pi^2)$ and

$$\Omega(w,w',m) = [\epsilon(w)/w^3]\theta(|w| - |w'| - m) \times [w^2 - 4ww' + w'^2 - m^2] \times \{[w^2 - (w'+m)^2][w^2 - (w'-m)^2]\}^{1/2} \tag{2.10a}$$

in the Feynman gauge, and

$$\Omega(w,w',m) = \tfrac{1}{2}[\epsilon(w)/w^3]\theta(|w| - |w'| - m)[(w-w')^2 - m^2] \times \{[w^2 - (w'+m)^2][w^2 - (w'-m)^2]\}^{1/2} \tag{2.10b}$$

in the Landau gauge. The expression (2.9) for $\Sigma(p)$ involves a convergent integral in both gauges, because of the Pauli–Villars cutoff.

In each gauge we substitute (2.9) into (2.5) and partially fractionate, obtaining

$$1 = \int_{-\infty}^{\infty} dw'\, \rho(w')\frac{\not p}{\not p - w'} - \lambda \int_{-\infty}^{\infty} dw'\, \rho(w') \times \int_{-\infty}^{\infty} dw'' \frac{\Omega(w'',w',m) - \Omega(w'',w',\Lambda)}{w'' - w'} \times \left[\frac{1}{\not p - w''} - \frac{1}{\not p - w'}\right]. \tag{2.11}$$

The imaginary part of this equation is

$$\phi(w)\rho(w) = \lambda \int_{-\infty}^{\infty} dw'\, \rho(w') \times \frac{\Omega(w,w',m) - \Omega(w,w',\Lambda)}{w - w'}, \tag{2.12}$$

where

$$\phi(w) = w + \lambda \int_{-\infty}^{\infty} dw' \frac{\Omega(w',w,m) - \Omega(w',w,\Lambda)}{w' - w}. \tag{2.13}$$

The function $\phi(w)$ may be calculated in closed form for either gauge. Equation (2.12) will be analyzed, in these gauges, in the next section.

III. ANALYSIS OF THE EQUATION

Equation (2.12) can be written

$$\phi(w)\rho(w) = \lambda\theta(|w| - m)\int_{-|w|+m}^{|w|-m} dw'\, \rho(w')\frac{\Omega(w,w',m)}{w - w'} - \lambda\theta(|w| - \Lambda)\int_{-|w|+\Lambda}^{|w|-\Lambda} dw'\, \rho(w')\frac{\Omega(w,w',\Lambda)}{w - w'}. \tag{3.1}$$

The θ functions are already implied by those in (2.10), they are included explicitly above to emphasize that the right-hand side of (3.1) vanishes when $|w| < m$.

First note that the denominator $w - w'$ never vanishes, and that the kernel in continuous. The function $\phi(w)$ is also bounded and continuous, and we may write

$$\phi(w)/w = 1 - \lambda\,[\psi(w,m) - \psi(w,\Lambda)], \tag{3.2}$$

where

$$\psi(w,m) = 2\int_{|w|+m}^{M} \frac{dw'}{w'^3} P(w'^2,w^2,m^2) \times \{[w'^2 - (w+m)^2][w'^2 - (w-m)^2]\}^{1/2} \tag{3.3}$$

with

$$P(w'^2,w^2,m^2) = 3 + (2w^2 + m^2)/(w'^2 - w^2) \tag{3.4a}$$

in the Feynman gauge, and

$$P(w'^2,w^2,m^2) = \tfrac{3}{2}(1 + m^2/(w'^2 - w^2)) \tag{3.4b}$$

in the Landau gauge. It is possible to express $\psi(w,m)$ in terms of elementary functions in both gauges. We have introduced a cutoff parameter M in the integral (3.3), which must be taken to infinity in (3.2). The integral in (3.3) diverges logarithmically as $M \to \infty$, but the function $\phi(w)$ in (3.2) is well defined in this limit. In particular,

$$\phi(w)/w \to 1 - b\lambda \log(\Lambda/m) \tag{3.5}$$

as $w \to 0$, where $b = 6$ in Feynman gauge and $b = 3$ in Landau gauge. In both gauges, $\phi(w)/w$ is monotonically increasing for $w > 0$ and

$$\phi(w)/w \to 1 \tag{3.6}$$

as $w \to \pm \infty$.

The odd function $\phi(w)$ is zero at $w = 0$. In addition, under the condition

$$\lambda > \lambda_c(\Lambda) = [b \log(\Lambda/m)]^{-1}, \tag{3.7}$$

it has a pair of zeros at $w = \pm w_0$, where w_0 is positive by convention. The function $\phi(w)$ has no positive zero for $\lambda < \lambda_c$. Note that the critical coupling $\lambda_c(\Lambda)$ goes to 0 as the Pauli–Villars cutoff parameter tends to infinity.

Let us consider Eq. (3.1). We know that any solution $\rho(w)$ vanishes for $|w| < m$. Furthermore, for $m \leqslant |w| < 2m$, the values of w' in the integrals on the right-hand side of (3.1) satisfy $|w'| < m$, for which $\rho(w')$ is 0. Consequently, $\rho(w)$ actually vanishes for $|w| < 2m$. In fact, one may iterate this procedure to show that $\rho(w)$ vanishes for all w. The conclusion is unavoidable if one requires the spectral density $\rho(w)$ to be a bounded continuous function. However, it is also possible for $\rho(w)$ to have delta distributions at those values of w for which $\phi(w)$ is 0; $\phi(w)\rho(w)$ and the integrals in (3.1) would then be ordinary functions.[12] Therefore, location of the zeros of $\rho(w)$ is a crucial ingredient in solving (3.1).

Let us set the mass scale by taking $m = 1$, and define the function

$$\lambda_0(w_0,\Lambda) = [\psi(w_0,1) - \psi(w_0,\Lambda)]^{-1}. \tag{3.8}$$

For coupling strength $\lambda = \lambda_0(w_0,\Lambda)$ with cutoff Λ, the function $\phi(\pm w_0)$ is 0, provided that λ_0 is greater than the critical coupling $\lambda_c(\Lambda)$; cf. Eq. (3.2). We find that $\lambda_0(w_0,\Lambda)$ is monotonically decreasing in w_0 for fixed Λ. The function $\lambda_0(w_0,\Lambda)$ is plotted against w_0 in Figs. 1(a) (Feynman gauge) and 1(b) (Landau gauge). Note that w_0 goes to 0 as λ approaches the critical coupling $\lambda_c(\Lambda)$ from above.

In Figs. 2(a) (Feynman gauge) and 2(b) (Landau gauge), w_0 is plotted against the cutoff parameter Λ for various choices of coupling strength λ_0. There is an approximate linear relation between Λ and w_0, which can be understood by examining the integral (3.3) in the parameter regime $M^2 \gg \Lambda^2 \gg w_0^2 \gg m^2 = 1$, to obtain

$$\psi(w_0,1) - \psi(w_0,\Lambda) \simeq 6 \log(\Lambda/w_0) + 2 \tag{3.9a}$$

in Feynman gauge, and

$$\psi(w_0,1) - \psi(w_0,\Lambda) \simeq 3 \log(\Lambda/w_0) - \tfrac{3}{4} \tag{3.9b}$$

in Landau gauge. Correspondingly, we get

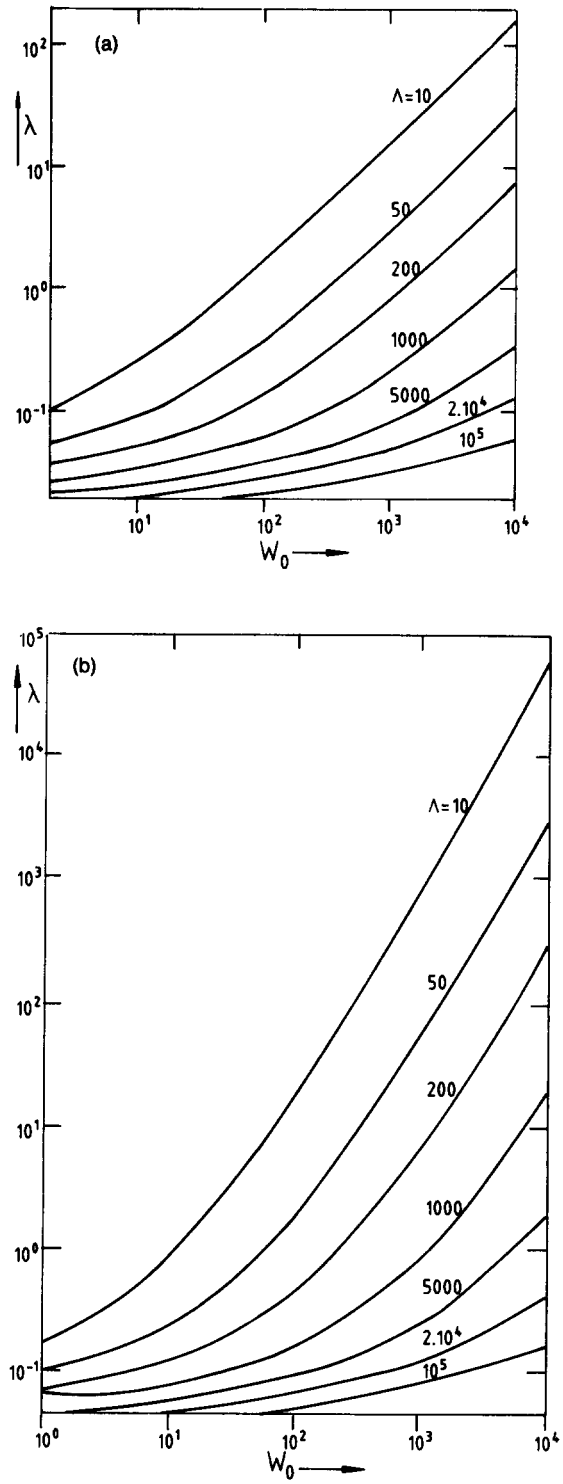

FIG. 1. λ_0 vs w_0 for various values of the cutoff Λ: (a) Feynman gauge, (b) Landau gauge.

$$\Lambda \simeq w_0 \exp\left[\frac{1}{b\lambda} + \frac{9 - 2b}{12}\right], \tag{3.10}$$

where b is 6 in Feynman gauge and 3 in Landau gauge, as in Eq. (3.5) above. These relations are valid to within a few percent for both gauges. Note, in particular, that for fixed λ, w_0 tends to infinity with Λ.

Let us look for solutions of Eq. (3.1) of the form

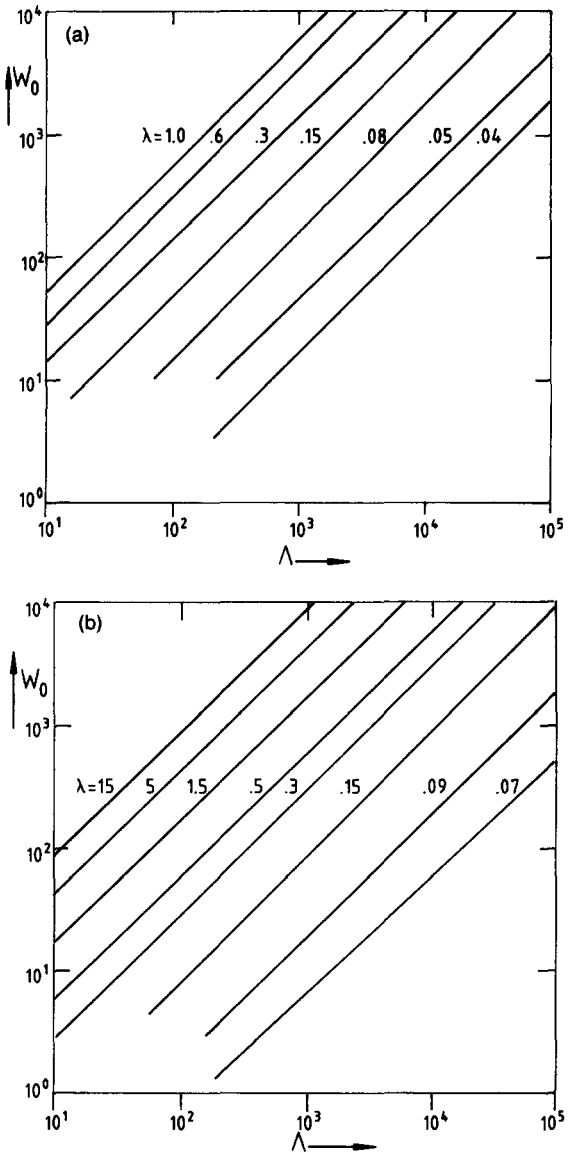

FIG. 2. w_0 versus cutoff parameter Λ for various values of coupling strength: (a) Feynman gauge, (b) Landau gauge.

$$\rho(w) = A\delta(w - w_0) + B\delta(w + w_0) + \sigma(w), \quad (3.11)$$

for constants A and B chosen arbitrarily, with the function $\sigma(w)$ to be determined. We obtain

$$\begin{aligned}\phi(w)\sigma(w) = {} & \lambda\theta(|w| - m - w_0)\left[A\frac{\Omega(w,w_0,m)}{w - w_0}\right. \\ & \left. + B\frac{\Omega(w,-w_0,m)}{w + w_0}\right] \\ & + \lambda\theta(|w| - m)\int_{-|w|+m}^{|w|-m} dw' \\ & \times\sigma(w')\frac{\Omega(w,w',m)}{w - w'} - [m\to\Lambda].\end{aligned} \quad (3.12)$$

The terms involving A and B vanish when $|w| < m + w_0$, and so $\sigma(w) = 0$ for $|w| < m + w_0$, by the argument given before. Hence we may replace $\theta(|w| - m)$ in Eq. (3.12) by $\theta(|w| - m - w_0)$. Indeed, it may be sharpened to $\theta(|w| - 2m - w_0)$, since $|w'|$ can exceed $m + w_0$ only when $|w| > 2m + w_0$. Now $\sigma(w)$ may be evaluated in successive steps of width m; for $m + w_0 < |w| < 2m + w_0$, it is given by just the first line of Eq. (3.12), for $2m + w_0 |w| < 3m + w_0$ the integral contributes, but it involves only the domain $m + w_0 < |w'| < 2m + w_0$, for which $\sigma(w')$ is already known, and so on. In short, Eq. (3.12) is not a true equation for $\sigma(w)$; it is rather a progressive algorithm for evaluating $\sigma(w)$ to arbitrarily large w values, and the existence of a solution, parametrized by A and B, is assured.

The solution implies the following Lehmann representation for the quark propagator:

$$\begin{aligned}S'_F(p) = {} & \frac{(A + B)\not{p} + (A - B)w_0}{p^2 - w_0^2} \\ & + \int_{\infty -}^{\infty} dw' \frac{\theta(|w'| - m - w_0)\sigma(w')}{\not{p} - w'}.\end{aligned} \quad (3.13)$$

There is a pole in the quark propagator at $p^2 = w_0^2$, but chiral symmetry actually remains unbroken when $A = B$. To verify the latter point, note that $\phi(w)$ is odd, the inhomogeneous term in (3.12) is an odd function of w when $A = B$, and the solution $\sigma(w)$ comes out as an even function of w. Thus the quark propagator (3.13) is proportional to $\not{p}$ and chiral symmetry is preserved. The choice $A \neq B$ leads to a propagator that breaks chiral symmetry.

In the continuum limit ($\Lambda \to \infty$), the pole in the quark propagator at $p^2 = w_0^2$ disappears to infinity. However, the parameters A and B can also be taken to depend upon Λ. In the continuum limit, the spectral density σ vanishes, and the renormalized quark propagator is of the form

$$S'_F(p) = a\not{p} + b. \quad (3.14)$$

The subtraction constants a and b, while not determined in the Salam–Delbourgo formalism, must be set to 0 on physical grounds. Consequently, only the trivial solution $S'_F(p) = 0$ survives in the continuum limit.

Finally, we turn to the zero of $\phi(w)$ at $w = 0$. There is another solution of (3.1) of the form

$$\rho(w) = \delta(w) + \sigma(w), \quad (3.15)$$

where $\sigma(w)$ satisfies Eq. (3.12) with replacements $w_0 = 0$ and $A + B = 1$. The inhomogeneous term in (3.12) is proportional to

$$\lambda\theta(|w| - m)\epsilon(w)(1 - m^2/w^2)^2 \quad (3.16)$$

in both gauges, and the solution $\sigma(w)$ is an even function of w. Consequently, the quark propagator becomes

$$S'_F(p) = \frac{\not{p}}{p^2} + 2\not{p}\int_m^{\infty} dw' \frac{\sigma(w')}{p^2 - w'^2}. \quad (3.17)$$

The quark propagator has a pole at $p^2 = 0$, and chiral symmetry remains unbroken at finite Λ, as well as in the continuum limit.

In summary, we have found two classes of solutions: in one class there may be a breaking of chiral symmetry with a cutoff present, but such solutions trivialize in the continuum limit; whereas the other class corresponds to unbroken chiral symmetry. Chiral symmetry thus remains unbroken

in the continuum limit in the Salam–Delbourgo formalism. These conclusions, which are established here in both Feynman and Landau gauges, are shown in Ref. 13 to apply also in the "Landau-like" gauge proposed by Maskawa and Nakajima in Ref. 2 and treated by us in Ref. 4.

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The concept of streamfunctions in the Wien effect on a weak electrolyte

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It is shown that streamfunctions $g^{(k)}$, $k = 1,2$, can be defined to describe the two ionic states of a weakly dissociated electrolyte in the presence of a uniform applied electric field. These states comprise the dissociated state and the associated state and the $g^{(k)}$ are shown to be governed by a second-order partial differential equation. By consideration of characteristic numbers describing the two ionic states this equation is solved using similarity solutions. The association rate constant and relative increase in the dissociation constant due to the applied electric field are shown to have simple expressions in terms of the $g^{(k)}$. It is suggested that the streamfunctions are more natural functions with which to describe the mathematical properties of a weak electrolyte than the corresponding distribution functions. Some important mathematical properties of the streamfunctions are discussed.

I. INTRODUCTION

Existing mathematical theories of the association and dissociation of a weak electrolyte in the presence of a uniform applied electric field **X** (Refs. 1 and 2), i.e., of the so-called Wien effect, are in terms of the distribution functions $f^{(k)}(r,\theta)$, $k = 1,2$, describing oppositely charged pairs of ions (i, j pairs), where r is the distance of separation of the ions in a pair and θ is the angle between **r** and **X**. The superscripts refer to the two ionic states that exist in weak electrolytes. These are the state of complete dissociation denoted by superscript 1 and the associated state denoted by superscript 2. In these theories solutions for the $f^{(k)}$ are sought from

$$\operatorname{div} f^{(k)}\mathbf{v}^{(k)} = 0 \tag{1.1}$$

that are the equations of continuity in the steady state of ionic flux, where $\mathbf{v}^{(k)}$ is the mean relative velocity of an i ion relative to the j ion of an i,j pair.

In Sec. II we discuss how the above-mentioned theories do not take full advantage of Eq. (1.1) by showing how these equations permit the introduction of the concept of streamfunctions $g^{(k)}(r,\theta)$ to describe the two ionic states of the weak electrolyte. Simple expressions for the association rate constant A and the relative increase in the dissociation constant $K(X)/K(0)$ are deduced in terms of the $g^{(k)}$. We derive the partial differential equation governing these streamfunctions in Sec. III and in Sec. IV we deduce possible characteristic numbers for the two ionic states of the weak electrolyte. These numbers are employed in Sec. V in solving by similarity solutions the governing partial differential equation for the $g^{(k)}$. Finally both A and $K(X)/K(0)$ are evaluated.

The originality of this work lies in the concept of the $g^{(k)}$ to describe the mathematical properties of a weak electrolyte, in the introduction of their governing partial differential equation, and in the solutions of this equation employing numbers characteristic of the weak electrolyte.

II. STREAMFUNCTIONS AND STREAMLINES

The law of mass action gives the equation for the time rate of change of associated ions in a weak electrolyte as

$$\frac{dv_{ij}}{dt} = An_in_j - KAv_{ij}, \tag{2.1}$$

where v_{ij} is the concentration of associated ions and n_i, n_j are the concentrations of dissociated ions. For a weak electrolyte $n_i,n_j \ll v_{ij}$, which implies, that although n_i, n_j are functions of the applied field intensity X, v_{ij} is independent of X.

In the steady state $dv_{ij}/dt = 0$ and the equation of continuity of ionic flux leads to Eq. (1.1).[3] The mean relative velocity of an i ion relative to a j ion is given by

$$\mathbf{v}^{(k)} = -\operatorname{grad}\Phi - (1/f^{(k)})\operatorname{grad} f^{(k)}, \quad k = 1,2, \tag{2.2}$$

where

$$\Phi = -1/r - 2\epsilon r\cos\theta \tag{2.3}$$

is the total electric potential of an i,j pair, $\epsilon = 2\beta q$,

$$\beta = \frac{(\omega_i e_i - \omega_j e_j)X}{2kT(\omega_i + \omega_j)}, \quad q = -\frac{e_i e_j}{2DkT} > 0,$$

where ω_i, ω_j are the mobility coefficients of the i, j ions, e_i, e_j their charges, k is Boltzmann's constant, T is absolute temperature, and D is the dielectric constant of the medium. To be specific we take $e_i > 0$ and $e_j < 0$ so that $\beta > 0$ and we take the origin at the position of the j ion of an i,j pair. In Eq. (2.3) the coordinate r and potential Φ have been nondimensionalized by division by the characteristic length $2q$ and by the characteristic potential kT, respectively. The i,j ions are assumed to be point ions and we further assume that the screening effects of the ionic atmospheres can be neglected in the region of interest which is the innermost region of the field of the ions. This is a valid assumption if n_i and n_j are sufficiently small to ensure that $\kappa^{-1} \gg q$, where

$$\kappa^{-1} = \{DkT/4\pi(n_i e_i^2 + n_j e_j^2)\}^{1/2}. \tag{2.4}$$

Here κ^{-1} is the Debye–Hückel radius of the ionic atmospheres and q is the Bjerrum association distance.

Since the flow pattern of ions in a weak electrolyte is clearly axisymmetric about the direction of **X** we suppose that there are functions $g^{(k)}$, $k = 1,2$, such that

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$$r^2 \sin\theta f^{(k)} v_r^{(k)} = -\frac{\partial g^{(k)}}{\partial \theta}, \quad r \sin\theta f^{(k)} v_\theta^{(k)} = \frac{\partial g^{(k)}}{\partial r}. \tag{2.5}$$

Evidently Eq. (1.1) is satisfied by this set and we call the $g^{(k)}(r,\theta)$ the *streamfunctions*. Similarly to the well-known definition of a streamfunction from fluid mechanics, $g^{(k)}$ has the following definition as a physical quantity: join a point Q, not coincident with the origin O, situated on the axis of symmetry $Z'OZ$ to a point P whose cordiantes are r,θ by a curve that lies in the plane of P and the axis. (See Fig. 1). In the steady state, the value of $2\pi g^{(k)}(r,\theta)$ at P is defined to be the average flux measured relative to O per unit time of i ions flowing across the surface of revolution generated by rotating the curve QP about $Z'OZ$. The positive direction of the flux is *away* from the axis.

The functions $g^{(k)}$ are clearly independent of the choice of the axial curve connecting Q to P and hence are functions of positions only. Furthermore, there is no average flux of i ions across the axis of symmetry and therefore the $g^{(k)}$ are independent of the position of Q on $Z'OZ$. When P coincides with Q the average flux of i ions relative to O will vanish and therefore

$$g(Q) = 0. \tag{2.6}$$

We will choose Q to be on the ray $\theta = \pi, r > 0$ and since there is no average flux of i ions across this ray, the $g^{(k)}$ are constant along $\theta = \pi$ and therefore from Eq. (2.6),

$$g^{(k)}(r,\pi) = 0, \quad 0 < r < \infty. \tag{2.7}$$

The streamfunctions lead naturally to the concept of *streamlines* for dissociated ions and associated ions: a streamline is a line in an axial plane that at any instant is everywhere parallel to the average relative velocity vector $\mathbf{v}^{(k)}$. The average flux of i ions across a streamline therefore vanishes and so along a streamline $g^{(k)}(r,\theta)$ can at most be a function of time. For a steady state this function of time must be a constant and the equation of a streamline reduces to

$$g^{(k)}(r,\theta) = \text{const}, \quad k = 1,2. \tag{2.8}$$

In the steady state the average flow field is the same for all time and a streamline defined by Eq. (2.8) therefore coincides with the average trajectory of an i ion relative to a j ion at O. The surface of revolution generated by a streamline rotated about the axis of symmetry is called a *streamsurface*. On a streamsurface, $g^{(k)} = \text{const}$. It is readily shown from Eq. (2.5) that

$$\mathbf{v}^{(k)} \cdot \text{grad}\, g^{(k)} = 0, \quad k = 1,2, \tag{2.9}$$

which confirms that the flow field lies on the streamsurface.

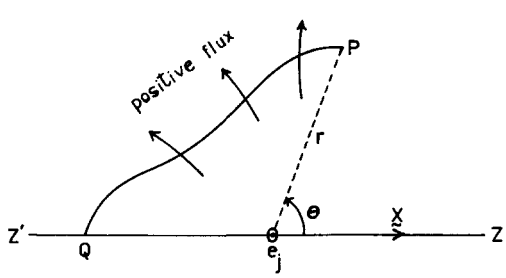

FIG. 1. Streamfunctions in a weak electrolyte.

The associaton rate constant and relative increase in the dissociation constant due to the applied electric field have very simple interpretations in terms of the streamfunctions. From Eq. (2.1),

$$An_i(X)n_j(X) = -\int_S f^{(1)}\mathbf{v}^{(1)} \cdot d\mathbf{S}, \tag{2.10}$$

where S is any closed surface completely surrounding the j ion at the origin. But the distribution function describing dissociated ions is the constant distribution[1] $f^{(1)}(r,\theta) = n_i(X)n_j(X)$ so on normalizing with respect to the characteristic distribution $n_i(X)n_j(X)$, $f^{(1)}(r,\theta) = 1$ and Eq. (2.10) gives

$$A = -\int_S \mathbf{v}^{(1)} \cdot d\mathbf{S}. \tag{2.11}$$

The association constant is independent of the choice of S.[3,4] If we therefore choose for S a closed surface of revolution generated by any axial curve joining any point Q not coincident with O on the ray $\theta = \pi$ and any point $P(r,0)$ with $r > 0$ on the ray $\theta = 0$, it follows immediately from the definition of $g^{(1)}$ that

$$A = -2\pi g^{(1)}(r,0). \tag{2.12}$$

Again from Eq. (2.1) on normalizing $f^{(2)}(r,\theta)$ by dividing by the constant distribution function $n_i(0)n_j(0)$,

$$\frac{K(X)}{K(0)} = \frac{1}{A}\int_S f^{(2)}\mathbf{v}^{(2)} \cdot d\mathbf{S}, \tag{2.13}$$

where S is any closed surface surounding the origin. From Eq. (1.1) it follows that $K(X)/K(0)$ is independent of the choice of S. We choose for S the closed surface of revolution chosen above for the association process. It follows from the definition of streamfunction that

$$K(X)/K(0) = (2\pi/A)g^{(2)}(r,0). \tag{2.14}$$

The simplicity of both Eqs. (2.12) and (2.14) lends strength to the view that the natural functions to describe the mathematical properties of the Wien effect on weak electrolytes are the streamfunctions $g^{(k)}$ rather than the distribution functions.

III. THE GOVERNING PARTIAL DIFFERENTIAL EQUATIONS

We next derive the partial differential equation governing $g^{(k)}(r,\theta)$ $k = 1,2$. From Eqs. (2.2), (2.3), and (2.5)

$$r^2 \sin\theta \frac{\partial f^{(k)}}{\partial r} - \frac{\partial g^{(k)}}{\partial \theta} + \sin\theta(1 - 2\epsilon r^2 \cos\theta) f^{(k)} = 0, \tag{3.1}$$

$$\sin\theta \frac{\partial f^{(k)}}{\partial \theta} + \frac{\partial g^{(k)}}{\partial r} + 2\epsilon r \sin^2\theta f^{(k)} = 0. \tag{3.2}$$

On eliminating $f^{(k)}$ from these equations we obtain

$$r^2 \frac{\partial^2 g^{(k)}}{\partial r^2} + \frac{\partial^2 g^{(k)}}{\partial \theta^2} + (1 - 2\epsilon r^2 \cos\theta)\frac{\partial g^{(k)}}{\partial r} + (2\epsilon r \sin\theta - \cot\theta)\frac{\partial g^{(k)}}{\partial \theta} = 0, \quad k = 1,2. \tag{3.3}$$

The boundary conditions for dissociated ions are

$$f^{(1)}(r,\theta) = 1, \tag{3.4}$$

$$g^{(1)}(r,\pi) = 0, \tag{3.5}$$

from Eq. (2.7) and for associated ions

$$\lim_{r\to 0} e^{-1/r} f^{(2)}(r,\theta) = 1, \tag{3.6}$$

$$\lim_{r\to\infty} f^{(2)}(r,\theta) = 0, \tag{3.7}$$

$$g^{(2)}(r,\pi) = 0, \tag{3.8}$$

from Eq. (2.7). Equation (3.6) is a manifestation of the Maxwell–Boltzmann equilibrium distribution at the distance of closest approach of an i,j pair and Eq. (3.7) represents the requirement that an i,j pair must be separated to infinity for complete dissociation.

IV. CHARACTERISTIC NUMBERS FOR WEAK ELECTROLYTES

The total electrical potential of an i,j pair is the sum of the Coulomb potential and the potential due to the applied electric field and is given by Eq. (2.3) that has the reference direction, θ_0, for potential, $\theta_0 = \pi/2$. For given values of ϵ and θ, Φ will attain a maximum value at $r = r_{\max}$, say, which is given by $r_{\max} = (2\epsilon\cos\theta)^{-1/2}$. The length $r_{\max}$ is finite $0 \leqslant \theta < \pi/2$ but is complex for $\pi/2 < \theta \leqslant \pi$ and would therefore not lead to a satisfactory characteristic length for the weak electrolyte.

This difficulty may be overcome by introducing an effective potential Φ_e given by

$$\Phi_e(r,\theta) = -1/r - \epsilon r(\cos\theta + 1), \tag{4.1}$$

which has the same value as Φ at $\theta = 0$ and has a maximum value for given values of ϵ and θ at $r = r_{\max}$, where

$$r_{\max} \triangleq (\epsilon(\cos\theta + 1))^{-1/2}. \tag{4.2}$$

The reference direction for Φ_e is $\Phi_e = \pi$, which, unlike the reference direction for Φ, has the virtue that it corresponds to a streamline for both associated and dissociated ions. With this definition $r_{\max}$ is finite for $0 \leqslant \theta < \pi$ having the minimum value of $(2\epsilon)^{-1/2}$ at $\theta = 0$ and increases monotonically as θ increases from 0. Thus Eq. (4.2) may lead to a suitable radial characteristic length $2qr_{\max}$ for the weak electrolyte. Accordingly we next transform the r coordinate

$$\bar{r} \triangleq r/r_{\max} = r(\epsilon y)^{1/2}, \tag{4.3}$$

where $y \triangleq 1 + \cos\theta$.

For *associated* ions we shall find that the function to work with is not $g^{(2)}(r,\theta)$ but is that obtained from this function by removing the factor $\exp[\epsilon y(y-2)]$. We therefore define $G(r,y)$ such that

$$G(r,y) \triangleq g^{(2)}(r,\theta)\exp[-\epsilon r(y-2)]. \tag{4.4}$$

If we similarly define

$$F(r,y) \triangleq f^{(2)}(r,\theta)\exp[-\epsilon r(y-2)], \tag{4.5}$$

then from Eq. (2.2)

$$\mathbf{v}^{(2)} = -\operatorname{grad}\Phi_e - (1/F)\operatorname{grad} F, \tag{4.6}$$

which shows that $F(r,y)$ is the distribution function associated with the potential Φ_e. Furthermore, from the first of Eqs. (2.5),

$$F\frac{\partial\Phi_e}{\partial r} + \frac{\partial F}{\partial r} = \frac{-\epsilon}{r}G - \frac{1}{r^2}\frac{\partial G}{\partial y}. \tag{4.7}$$

If we make the assumption that F is an equilibrium distribution $F \propto \exp(-\Phi_e)$, and Eq. (4.7) gives $\partial G/\partial y = -G/(y/\epsilon)^{1/2}$ when $r = r_{\max}$. This implies that a suitable characteristic number for the y coordinate may be

$$y_{\text{ch}} = (y/\epsilon)^{1/2} \tag{4.8}$$

and thus for dissociating ions we obtain a coordinate companion to $\bar{r}$ as

$$\bar{y} \triangleq y/y_{\text{ch}} = (\epsilon y)^{1/2}. \tag{4.9}$$

V. SOLUTIONS FOR THE STREAMFUNCTIONS

On setting $g^{(k)}(r,\theta) = h^{(k)}(r,y)$, Eq. (3.3) becomes

$$r^2\frac{\partial^2 h^{(k)}}{\partial r^2} + y(2-y)\frac{\partial^2 h^{(k)}}{\partial y^2} + (1 - 2\epsilon r^2(y-1))\frac{\partial h^{(k)}}{\partial r} - 2\epsilon r y(2-y)\frac{\partial h^{(k)}}{\partial y} = 0, \quad k = 1,2. \tag{5.1}$$

A. Dissociated ions

The boundary conditions (3.4) and (3.5) become

$$f^{(1)}(r,\theta) = 1, \tag{5.2}$$

$$h^{(1)}(r,0) = 0. \tag{5.3}$$

We shall solve Eq. (5.1) for $h^{(1)}(r,y)$ using the similarity transformation indicated by Eq. (4.3). By writing

$$h^{(1)}(r,y) = H^{(1)}(\bar{r},y), \tag{5.4}$$

Eq. (5.1) gives

$$\frac{\bar{r}^2(2+3y)}{4y}\frac{\partial^2 H^{(1)}}{\partial\bar{r}^2} + \left(\frac{-\bar{r}(2-y)}{4y} + (\epsilon y)^{1/2}(1-\bar{r}^2)\right)\frac{\partial H^{(1)}}{\partial\bar{r}} + \bar{r}(2-y)\frac{\partial^2 H^{(1)}}{\partial\bar{r}\,\partial y} + y(2-y)\frac{\partial^2 H^{(1)}}{\partial y^2} - 2(\epsilon y)^{1/2}\bar{r}(2-y)\frac{\partial H^{(1)}}{\partial y} = 0. \tag{5.5}$$

This equation is similar to the example discussed by Hansen[5]: if we set

$$H^{(1)}(\bar{r},y) = F(\bar{r})(2-y), \tag{5.6}$$

Eq. (5.5) gives

$$\frac{\bar{r}^2(2+3y)}{4y}F'' + \left(\frac{-\bar{r}(2+3y)}{4y} + (\epsilon y)^{1/2}(1-\bar{r}^2)\right)F' + 2(\epsilon y)^{1/2}\bar{r}F = 0, \tag{5.7}$$

which possesses only one solution, $F(\bar{r}) = 1 - \bar{r}^2$, analytic at the irregular singular point $\bar{r} = 0$. Thus $H^{(1)}(\bar{r},y) = (1-\bar{r}^2)(2-y)$ is a solution of Eq. (5.5) and the required solution of this equation is therefore

$$H^{(1)}(\bar{r},y) = B_1(1-\bar{r}^2)(2-y) + B_2, \tag{5.8}$$

where B_1 and B_2 are constants. The corresponding solution of Eq. (5.1) is

$$h^{(1)}(r,y) = B_1(1-\epsilon r^2 y)(2-y) + B_2. \tag{5.9}$$

The boundary condition (5.3) requires that $B_2 = -2B_1$, and from Eq. (3.1) or (3.2) and Eq. (5.2) we find that $B_1 = 1$ and so

$$h^{(1)}(r,y) = (1 - \epsilon r^2 y)(2 - y) - 2 \tag{5.10}$$

and

$$g^{(1)}(r,\theta) = -(1 + \cos\theta)(1 + \epsilon r^2(1 - \cos\theta)) \tag{5.11}$$

is the streamfunction describing dissociated ions.

Next consider the way in which association depends on the angle of association. From the definition, $2\pi g^{(1)}(r,\theta)$ is the averge flux of i ions in a direction away from the axis of symmetry across the surface of revolution generated by any axial curve joining the reference point Q on the ray $\theta = \pi$ to the point $P(r,\theta)$. This flux depends on r and θ since the surface is not closed. Let us constrain P to vary only along a streamline that intersects the origin. Then since $g^{(1)}$ is constant along a streamline $g^{(1)}(r,\theta) = g^{(1)}(0,\alpha)$, where α is the angle which the streamline makes with X at $r = 0$, $0 \leqslant \alpha \leqslant \pi$. If we define $\overline{A}(\alpha)$ to be the average association flux across the surface of revolution generated by any axial curve joining Q to any point P on the streamline making angle α with X at $r = 0$, then

$$\overline{A}(\alpha) = -2\pi g^{(2)}(0,\alpha) = 2\pi(1 + \cos\alpha) \tag{5.12}$$

from Eqs. (2.12) and (5.11). Here $\overline{A}(\alpha)$ increases monotonically as α decreases from π to 0, which is consistent with the existence of a sink singularity at $r = 0$. We note that $\overline{A}(\alpha)$ is independent of ϵ, which is a generalization of Langevin's theorem[4] that states that the association constant A is independent of ϵ. From Eqs. (2.12) and (5.11), or Eq. (5.12),

$$A = \overline{A}(0) = 4\pi. \tag{5.13}$$

B. Associated Ions

We have to solve Eq. (5.1) with $k = 2$ subject to boundary conditions (3.6), (3.7), and Eq. (3.8) becomes

$$h^{(2)}(r,0) = 0. \tag{5.14}$$

We first observe that if we define $p(r,y)$ by

$$h^{(2)}(r,y) = p(r,y)\exp[\epsilon r(y - 1)], \tag{5.15}$$

Eq. (5.1) is rendered in separable form,

$$r^2\frac{\partial^2 p}{\partial r^2} + \frac{\partial p}{\partial r} - \epsilon^2 r^2 p = -y(2 - y)\frac{\partial^2 p}{\partial y^2} - \epsilon(y - 1)p, \tag{5.16}$$

which on setting $p(r,y) = R(r)Y(y)$ gives

$$\begin{aligned} r^2\frac{d^2R}{dr^2} + \frac{dR}{dr} - (\epsilon^2 r^2 + \lambda)R &= 0, \\ y(2 - y)\frac{d^2y}{dy^2} + (\epsilon(y - 1) + \lambda)Y &= 0, \end{aligned} \tag{5.17}$$

where λ is the separation constant. Thus

$$\frac{d^2R}{dr^2} + \frac{1}{r^2}\frac{dR}{dr} - \epsilon^2 R = 0 \quad \text{as } r \to \infty, \tag{5.18}$$

from which

$$R \sim C_1 e^{\epsilon r} + C_2 e^{-\epsilon r} \quad \text{as } r \to \infty, \tag{5.19}$$

where C_1 and C_2 are constants. But $\lim_{r\to\infty} rf^{(2)}(r,\theta) = \exp[\epsilon r(\cos\theta - 1)]$ (Ref. 6) and so from Eq. (3.2) C_1 must be 0 giving

$$h^{(2)}(r,y) \sim \exp[\epsilon r(y - 2)] \text{ as } r \to \infty. \tag{5.20}$$

Since this function depends *explicitly* on ϵ when we transform to the coordinates $\bar{r}, \bar{y}$ defined by Eqs. (4.3) and (4.9), we define $H^{(2)}(\bar{r},\bar{y})$ by

$$h^{(2)}(r,y) \triangleq H^{(2)}(\bar{r},\bar{y})\exp[\epsilon r(y - 2)], \tag{5.21}$$

whence Eq. (5.1) gives

$$\begin{aligned} &\frac{\bar{r}^2}{\bar{y}^2}\frac{\partial^2 H^{(2)}}{\partial \bar{r}^2} - \left(\frac{\bar{r}}{2\bar{y}^2} + \frac{2\bar{r}^2}{\bar{y}}\right)\frac{\partial H^{(2)}}{\partial \bar{r}} + \frac{\bar{r}}{\bar{y}}\frac{\partial^2 H^{(2)}}{\partial \bar{r}\,\partial \bar{y}} \\ &\quad - \frac{1}{2\bar{y}}\frac{\partial H^{(2)}}{\partial \bar{y}} + \frac{1}{2}\frac{\partial^2 H^{(2)}}{\partial \bar{y}^2} - 2H^{(2)} \\ &\quad + \epsilon^{-1}\left\{\frac{3}{4}\bar{r}^2\frac{\partial^2 H^{(2)}}{\partial \bar{r}^2} + \left(\bar{y} + \frac{\bar{r}}{4}\right)\frac{\partial H^{(2)}}{\partial \bar{r}}\right. \\ &\quad - \frac{\bar{r}\bar{y}}{2}\frac{\partial^2 H^{(2)}}{\partial \bar{r}\,\partial \bar{y}} \\ &\quad \left. + \frac{\bar{y}}{4}\frac{\partial H^{(2)}}{\partial \bar{y}} - \frac{\bar{y}^2}{4}\frac{\partial^2 H^{(2)}}{\partial \bar{y}^2} + \bar{y}^2 H^{(2)}\right\} = 0. \end{aligned} \tag{5.22}$$

If we further assume that $H^{(2)}(\bar{r},\bar{y})$ is not an explicit function of ϵ then we must have

$$\begin{aligned} &\frac{\bar{r}^2}{2\bar{y}^2}\frac{\partial^2 H^{(2)}}{\partial \bar{r}^2} - \left(\frac{\bar{r}}{2\bar{y}^2} + \frac{2\bar{r}^2}{\bar{y}}\right)\frac{\partial H^{(2)}}{\partial \bar{r}} + \frac{\bar{r}}{\bar{y}}\frac{\partial^2 H^{(2)}}{\partial \bar{r}\partial \bar{y}} \\ &\quad - \frac{1}{2\bar{y}}\frac{\partial H^{(2)}}{\partial \bar{y}} + \frac{1}{2}\frac{\partial^2 H^{(2)}}{\partial \bar{y}^2} - 2H^{(2)} = 0 \end{aligned} \tag{5.23}$$

and

$$\begin{aligned} &\frac{3}{4}\bar{r}^2\frac{\partial^2 H^{(2)}}{\partial \bar{r}^2} + \left(\bar{y} + \frac{\bar{r}}{4}\right)\frac{\partial H^{(2)}}{\partial \bar{r}} - \frac{\bar{r}\bar{y}}{2}\frac{\partial^2 H^{(2)}}{\partial \bar{r}\,\partial \bar{y}} \\ &\quad + \frac{\bar{y}}{4}\frac{\partial H^{(2)}}{\partial \bar{y}} - \frac{\bar{y}^2}{4}\frac{\partial^2 H^{(2)}}{\partial \bar{y}^2} + \bar{y}^2 H^{(2)} = 0. \end{aligned} \tag{5.24}$$

First consider Eq. (5.23), which is a parabolic equation whose characteristic directions are given by

$$\frac{\bar{r}^2}{\bar{y}^2}\left(\frac{d\bar{y}}{d\bar{r}}\right)^2 - \frac{2\bar{r}}{\bar{y}}\frac{d\bar{y}}{d\bar{r}} + 1 = 0, \tag{5.25}$$

and which has the solution $\bar{y} = \text{const}\,\bar{r}$. We therefore define the canonical coordinates

$$\xi(\bar{r},\bar{y}) = \bar{y}/\bar{r}, \quad \eta = \eta(\bar{r},\bar{y}), \tag{5.26}$$

and $q(\xi,\eta) = H^{(2)}(\bar{r},\bar{y})$ and Eq. (5.24) becomes

$$\begin{aligned} &\left(\frac{\bar{r}^2}{2\bar{y}^2}\left(\frac{\partial \eta}{\partial \bar{r}}\right)^2 + \frac{\bar{r}}{\bar{y}}\frac{\partial \eta}{\partial \bar{r}}\frac{\partial \eta}{\partial \bar{y}} + \frac{1}{2}\left(\frac{\partial \eta}{\partial \bar{y}}\right)^2\right)\frac{\partial^2 q}{\partial \eta^2} \\ &\quad + 2\frac{\partial q}{\partial \xi} + \left(\frac{\bar{r}^2}{2\bar{y}^2}\frac{\partial^2 \eta}{\partial \bar{r}^2} - \left[\frac{\bar{r}}{2\bar{y}^2} + \frac{2\bar{r}^2}{\bar{y}}\right]\frac{\partial \eta}{\partial \bar{r}}\right. \\ &\quad \left. + \frac{\bar{r}}{\bar{y}}\frac{\partial^2 \eta}{\partial \bar{r}\,\partial \bar{y}} - \frac{1}{2\bar{y}}\frac{\partial \eta}{\partial \bar{y}} - \frac{1}{2}\frac{\partial^2 \eta}{\partial \bar{y}^2}\right)\frac{\partial q}{\partial \eta} - 2q = 0. \end{aligned} \tag{5.27}$$

For a parabolic equation the choice of $\eta(\bar{r},\bar{y})$ is arbitrary. If we take $\eta = \bar{y}$, Eq. (5.27) reduces to

$$\frac{\partial^2 q}{\partial \bar{y}^2} - \frac{1}{\bar{y}}\frac{\partial q}{\partial \bar{y}} + 4\frac{\partial q}{\partial \xi} - 4q = 0, \tag{5.28}$$

and on setting $q(\xi,\bar{y}) = Z(\xi)Y(\bar{y})$ in this equation we obtain

$$\frac{d^2Y}{d\bar{y}^2} - \frac{1}{\bar{y}}\frac{dY}{d\bar{y}} - \gamma Y = 0 \tag{5.29}$$

and

$$4\frac{dZ}{d\xi} + (\gamma - 4)Z = 0, \tag{5.30}$$

where γ is the separation constant.

Equation (5.29) is solved by setting $Y(\bar{y}) = \bar{y}W(\bar{y})$ and it then becomes

$$\bar{y}^2\frac{d^2W}{d\bar{y}^2} + \bar{y}\frac{dW}{d\bar{y}} - (1 + \gamma\bar{y}^2)W = 0, \tag{5.31}$$

which has the solution

$$W(\bar{y}) = \text{const}_1\, I_1(\gamma^{1/2}\bar{y}) + \text{const}_2\, K_1(\gamma^{1/2}\bar{y}), \tag{5.32}$$

where I_1, K_1 are, respectively, the modified Bessel function of the first kind and modified Bessel function of the second kind both of order 1. Equation (5.30) has the solution

$$Z(\xi) = \text{const}\exp[(1 - \gamma/4)\xi], \tag{5.33}$$

and thus the solution of Eq. (5.23) is

$$H^{(2)}(\bar{r},\bar{y}) = \bar{y}\exp[(1 - \gamma/4)\bar{y}/\bar{r}](D_1 I_1(\gamma^{1/2}\bar{y}) + D_2 K_1(\gamma^{1/2}\bar{y})), \tag{5.34}$$

where D_1 and D_2 are constants. However $\bar{y}I_1(\gamma^{1/2}\bar{y}) = O(\bar{y}^2)$ as $\bar{y}\to 0$ and $\bar{y}K_1(\gamma^{1/2}\bar{y}) = O(\gamma^{-1/2})$ as $\bar{y}\to 0$ so in order to satisfy the boundary condition (5.14) we must have $D_2 = 0$ so that

$$H^{(2)}(\bar{r},\bar{y}) = D_1\bar{y}\exp[(1 - \gamma/4)\bar{y}/\bar{r}]I_1(\gamma^{1/2}\bar{y}). \tag{5.35}$$

Furthermore this solution satisfies Eq. (5.24) if and only if $\gamma = 4$. Thus the required solution to Eq. (5.22) is

$$H^{(2)}(\bar{r},\bar{y}) = D_1\bar{y}I_1(2\bar{y}), \tag{5.36}$$

or in terms of the r,θ coordinates the required solution to Eq. (3.3) is

$$g^{(2)}(r,\theta) = D_1(2\epsilon)^{1/2}\cos(\theta/2)I_1((8\epsilon)^{1/2}\cos(\theta/2)) \times\exp[\epsilon r(\cos\theta - 1)]. \tag{5.37}$$

The final problem in determining $g^{(2)}(r,\theta)$ is to evaluate D_1. We have, from Eqs. (3.1), (3.2), and (5.37) using the identity[7] $xI_1'(x) = -I_1(x) + xI_0(x)$,

$$\frac{\partial f^{(2)}}{\partial r} + \left(\frac{1}{r^2} - 2\epsilon\cos\theta\right)f^{(2)} = -D_1(2\epsilon)^{1/2}\left\{\frac{(2\epsilon)^{1/2}}{2r^2}I_0\left((8\epsilon)^{1/2}\cos\frac{\theta}{2}\right) + \frac{\epsilon}{r}\cos\frac{\theta}{2}I_1\left((8\epsilon)^{1/2}\cos\frac{\theta}{2}\right)\right\} \times\exp[\epsilon r(\cos\theta - 1)], \tag{5.38}$$

$$\frac{\partial f^{(2)}}{\partial\theta} + 2\epsilon r\sin\theta f^{(2)} = D_1 2^{1/2}\epsilon^{3/2}\sin\frac{\theta}{2}I_1\left((8\epsilon)^{1/2}\cos\frac{\theta}{2}\right) \times\exp[\epsilon r(\cos\theta - 1)]. \tag{5.39}$$

Next consider the Pfaffian differential equation arising from this pair of equations. This is

$$df^{(2)} = \left\{\left(-\frac{1}{r^2} + 2\epsilon\cos\theta\right)f^{(2)} - D_1(2\epsilon)^{1/2}\left[\frac{(2\epsilon)^{1/2}}{2r^2}I_0\left((8\epsilon)^{1/2}\cos\frac{\theta}{2}\right) + \frac{\epsilon}{r}\cos\frac{\theta}{2}I_1\left((8\epsilon)^{1/2}\cos\frac{\theta}{2}\right)\right] \times\exp[\epsilon r(\cos\theta - 1)]\right\}dr + \left\{-2\epsilon r\sin\theta f^{(2)} + D_1 2^{1/2}\epsilon^{3/2}\sin\frac{\theta}{2} \times I_1\left((8\epsilon)^{1/2}\cos\frac{\theta}{2}\right)\exp[\epsilon r(\cos\theta - 1)]\right\}d\theta. \tag{5.40}$$

This equation is shown to be integrable in the Appendix. We integrate using the method of Natani.[8] First we treat the variable r as a constant and solve the resulting differential equation. Taking r as a constant, Eq. (5.40) becomes

$$\frac{df^{(2)}}{d\theta} + 2\epsilon r\sin\theta f^{(2)} = D_1 2^{1/2}\epsilon^{3/2}\sin\frac{\theta}{2}I_1\left((8\epsilon)^{1/2}\cos\frac{\theta}{2}\right) \times\exp[\epsilon r(\cos\theta - 1)], \tag{5.41}$$

which implies that

$$f^{(2)}(r,\theta) = \exp[2\epsilon r\cos\theta]\left\{D_1 2^{1/2}\epsilon^{3/2}\int\sin\frac{\theta}{2} \times I_1\left((8\epsilon)^{1/2}\cos\frac{\theta}{2}\right) \times\exp[-\epsilon r(\cos\theta + 1)]d\theta + D_3(r)\right\}, \tag{5.42}$$

where $D_3(r)$ is a function of r only.

The right-hand side of Eq. (5.42) may be integrated by the substitution

$$u = (8\epsilon)^{1/2}\cos(\theta/2) \tag{5.43}$$

and the identity

$$\frac{d}{du}(u^{n+1}I_{n+1}(u)) = u^{n+1}I_n(u) \tag{5.44}$$

for modified Bessel functions I_n of the first kind of order n. We find that

$$-(2\epsilon)^{1/2}\int\sin\frac{\theta}{2}I_1\left((8\epsilon)^{1/2}\cos\frac{\theta}{2}\right) \times\exp[-\epsilon r(\cos\theta + 1)]d\theta = e^{-ru^2/4}\left(I_0(u) + \frac{ru}{2}I_1(u) + \left(\frac{ru}{2}\right)^2 I_2(u) + \cdots + \left(\frac{ru}{2}\right)^n I_n(u)\right) + R_n(u), \tag{5.45}$$

where

$$R_n(u) = \left(\frac{r}{2}\right)^{n+1}\int u^{n+1}I_n(u)e^{-ru^2/4}\,du. \tag{5.46}$$

The remainder can be evaluated as follows. Using the expansion

$$I_n(u) = \sum_{s=0}^{\infty} \frac{1}{s!(n+s)!}\left(\frac{u}{2}\right)^{n+2s} \tag{5.47}$$

and making the change of variable $v = ru^2/4$ we have

$$R_n = \sum_{s=0}^{\infty} \frac{1}{s!(n+s)!r^s} \int v^{n+s} e^{-v}\, dv. \tag{5.48}$$

But by successive integration by parts

$$\int v^{n+s} e^{-v}\, dv = -e^{-v}(n+s)! \sum_{p=0}^{n+s} \frac{v^p}{p!} \tag{5.49}$$

and so

$$R_n = -e^{-v} \sum_{s=0}^{\infty} \frac{1}{s!r^s} \sum_{p=0}^{n+s} \frac{v^p}{p!} \tag{5.50}$$

and

$$\lim_{n\to\infty} R_n = -\sum_{s=0}^{\infty} \frac{1}{s!r^s} = -e^{1/r}. \tag{5.51}$$

Thus

$$\begin{aligned} &-(2\epsilon)^{1/2} \int \sin\frac{\theta}{2} I_1\left((8\epsilon)^{1/2}\cos\frac{\theta}{2}\right) \\ &\quad \times \exp[-\epsilon r(\cos\theta + 1)]\, d\theta \\ &\quad = \exp[-\epsilon r(\cos\theta + 1)] \sum_{p=0}^{\infty} \left(\frac{r(8\epsilon)^{1/2}\cos(\theta/2)}{2}\right)^p \\ &\quad \times I_p\left((8\epsilon)^{1/2}\cos\frac{\theta}{2}\right) - e^{1/r}, \end{aligned} \tag{5.52}$$

and Eq. (5.42) therefore gives

$$\begin{aligned} &f^{(2)}(r,\theta) \\ &\quad = -D_1\epsilon \exp[\epsilon r(\cos\theta - 1)] \\ &\qquad \times \sum_{p=0}^{\infty} \left(\frac{r(8\epsilon)^{1/2}\cos(\theta/2)}{2}\right)^p \\ &\qquad \times I_p\left((8\epsilon)^{1/2}\cos\frac{\theta}{2}\right) + D_1\epsilon \exp\left[\frac{1}{r} + 2\epsilon r\cos\theta\right] \\ &\qquad + D_3(r)\exp(2\epsilon r\cos\theta). \end{aligned} \tag{5.53}$$

We next set $\theta = \pi$ in Eq. (5.40), which becomes

$$\frac{df^{(2)}}{dr} + \left(\frac{1}{r^2} + 2\epsilon\right) f^{(2)} = -\frac{D_1\epsilon}{r^2}\exp(-2\epsilon r), \tag{5.54}$$

and which has the solution

$$f^{(2)}(r,\pi) = -D_1\epsilon \exp(-2\epsilon r) + D_4 \exp(1/r - 2\epsilon r), \tag{5.55}$$

where D_4 is constant because θ has been given the *definite* value of $\theta = \pi$. Comparing Eq. (5.53) with $\theta = \pi$ and Eq. (5.55) gives

$$D_3(r) = (D_4 - \epsilon D_1)e^{1/r} \tag{5.56}$$

and so

$$\begin{aligned} f^{(2)}(r,\theta) = &-D_1\epsilon \exp[\epsilon r(\cos\theta - 1)] \\ &\times \sum_{p=0}^{\infty} \left(\frac{r(8\epsilon)^{1/2}\cos(\theta/2)}{2}\right)^p I_p\left((8\epsilon)^{1/2}\cos\frac{\theta}{2}\right) \\ &+ D_4 \exp\left(\frac{1}{r} + 2\epsilon r\cos\theta\right) \end{aligned} \tag{5.57}$$

and the boundary condition at $r = 0$ [Eq. (3.6)] therefore gives $D_4 = 1$.

To determine D_1 we have first the identity[8]

$$\exp\left[\frac{x}{2}\left(s + \frac{1}{s}\right)\right] = \sum_{n=-\infty}^{\infty} s^n I_n(x). \tag{5.58}$$

Taking $x = (8\epsilon)^{1/2}\cos(\theta/2)$, $s = r(8\epsilon)^{1/2}\cos(\theta/2)/2$, Eq. (5.58) gives

$$\begin{aligned} &\sum_{n=0}^{\infty} \left(\frac{r(8\epsilon)^{1/2}\cos(\theta/2)}{2}\right)^n I_n\left((8\epsilon)^{1/2}\cos\frac{\theta}{2}\right) \\ &\quad = -\sum_{n=1}^{\infty} \left(\frac{2}{r(8\epsilon)^{1/2}\cos(\theta/2)}\right)^n I_n\left((8\epsilon)^{1/2}\cos\frac{\theta}{2}\right) \\ &\qquad + \exp\left[\frac{1}{r} + \epsilon r(\cos\theta + 1)\right] \end{aligned} \tag{5.59}$$

and using this with $D_4 = 1$ Eq. (5.57) becomes

$$\begin{aligned} f^{(2)}(r,\theta) = &D_1\epsilon \exp[\epsilon r(\cos\theta - 1)] \\ &\times \sum_{n=1}^{\infty} \left(\frac{2}{r(8\epsilon)^{1/2}\cos(\theta/2)}\right)^n \\ &\times I_n\left((8\epsilon)^{1/2}\cos\frac{\theta}{2}\right) \\ &+ (1 - \epsilon D_1)\exp\left(\frac{1}{r} + 2\epsilon r\cos\theta\right) \end{aligned} \tag{5.60}$$

and the boundary condition (3.7) therefore requires that $D_1 = 1/\epsilon$ and so from Eqs. (5.37) and (5.57),

$$\begin{aligned} f^{(2)}(r,\theta) = &-\exp[\epsilon r(\cos\theta - 1)] \\ &\times \sum_{p=0}^{\infty} \left(\frac{r(8\epsilon)^{1/2}\cos(\theta/2)}{2}\right)^p \\ &\times I_p\left((8\epsilon)^{1/2}\cos\frac{\theta}{2}\right) \\ &+ \exp\left(\frac{1}{r} + 2\epsilon r\cos\theta\right) \end{aligned} \tag{5.61}$$

and

$$\begin{aligned} g^{(2)}(r,\theta) = &\left(\frac{2}{\epsilon}\right)^{1/2} \cos\frac{\theta}{2} I_1\left((8\epsilon)^{1/2}\cos\frac{\theta}{2}\right) \\ &\times \exp[\epsilon r(\cos\theta - 1)]. \end{aligned} \tag{5.62}$$

The equivalence of Eq. (5.61) and Onsager's expression[1]

$$\begin{aligned} f^{(2)}(r,\theta) = &\frac{1}{r}\exp\left[\frac{1}{r} + \epsilon r(\cos\theta - 1)\right] \\ &\times \int_0^1 I_0\left((8\epsilon)^{1/2}\cos\frac{\theta}{2}\right) e^{-s/r}\, ds \end{aligned} \tag{5.63}$$

may be easily demonstrated. Furthermore from Eqs. (2.14) and (5.13), Eq. (5.62) gives

$$\frac{K(X)}{K(0)} = \frac{1}{2} g^{(2)}(r,0) = \frac{I_1[(8\epsilon)^{1/2}]}{(2\epsilon)^{1/2}}, \tag{5.64}$$

which is Onsager's well-known result.

We further observe that since $\xi = \bar{y}/\bar{r} = 1/r$, the transformation $\bar{r} = r(\epsilon y)^{1/2}$ is unnecessary in the above analysis. The only necessary transformation is $\bar{y} = (\epsilon y)^{1/2}$, which suggests that the characteristic length for associated ions is the transverse length $2qy_{ch}r_{max} = 2q/\epsilon$.

Finally, the following important deduction may be made from Eq. (5.62). Let us define $4\pi\bar{K}(\theta_0;\epsilon)$ as the aver-

age flux of i ions away from the axis across the surface of revolution generated by any axial curve joining the reference point Q on the ray $\theta=\pi$ to any point P on the streamline that makes an angle θ_0 with X at $r=0$. Suppose that P is constrained to vary only along this streamline. Since $g^{(2)}$ is constant along a streamline $g^{(2)}(P)=g^{(2)}(0,\theta_0)$ and therefore

$$\begin{aligned}\overline{K}(\theta_0;\epsilon) &= \tfrac{1}{2}g^{(2)}(0,\theta_0)\\ &= \cos(\theta_0/2)I_1[(8\epsilon)^{1/2}\cos(\theta_0/2)]/(2\epsilon)^{1/2}.\end{aligned} \tag{5.65}$$

The function $\overline{K}(\theta_0;\epsilon)$ increases monotonically from 0 to $K(X)/K(0)$ as θ_0 decreases from π to 0, which is consistent with the existence of a *source* (for associated ions) at the origin; $\overline{K}(\theta_0;\epsilon)$ is the contribution to $K(X)/K(0)$ made by those trajectories emanating from the origin at angles from $\theta=\pi$ to $\theta=\theta_0$. The fractional contribution ν of this range of "initial angles" compared to $K(X)/K(0)$ is from Eqs. (5.64) and (5.65) given by

$$\nu=\cos(\theta_0/2)I_1[(8\epsilon)^{1/2}\cos(\theta_0/2)]/I_1[(8\epsilon)^{1/2}]. \tag{5.66}$$

Of special interest is the value of ν, where $\theta_0=\pi/2$. In this case $\nu=49.75\%$ when $\epsilon=0.01$ and $\nu=6\%$ when $\epsilon=10$. This shows that when the applied field intensity is very small the contribution to dissociation by the forward directions ($\theta_0<\pi/2$) is approximately equal to the contribution made by the reverse angles ($\theta_0>\pi/2$) but that when the applied field intensity is large, the contribution to dissociation made by the forward directions is much greater than the contribution made by the reverse directions.

APPENDIX: INTEGRABILITY OF THE PFAFFIAN DIFFERENTIAL EQUATION

We have from Eqs. (5.38) and (5.39),

$$\begin{aligned}df^{(2)} &= \frac{\partial f^{(2)}}{\partial r}(f^{(2)},r,\theta)dr+\frac{\partial f^{(2)}}{\partial\theta}(f^{(2)},r,\theta)d\theta\\ &= P(f^{(2)},r,\theta)dr+Q(f^{(2)},r,\theta)d\theta,\end{aligned} \tag{A1}$$

say, where

$$\begin{aligned}P(f^{(2)},r,\theta) = {}& (-1/r^2+2\epsilon\cos\theta)f^{(2)}\\ &-D_1(2\epsilon)^{1/2}\exp[\epsilon r(\cos\theta-1)]\\ &\times\{[(2\epsilon)^{1/2}/2r^2]I_0((8\epsilon)^{1/2}\cos(\theta/2))\\ &+(\epsilon/r)\cos(\theta/2)I_1[(8\epsilon)^{1/2}\cos(\theta/2)]\}\end{aligned} \tag{A2}$$

and

$$\begin{aligned}Q(f^{(2)},r,\theta) = {}& -2\epsilon r\sin\theta f^{(2)}\\ &+D_1 2^{1/2}\epsilon^{3/2}\exp[\epsilon r(\cos\theta-1)]\\ &\times\sin(\theta/2)I_1[(8\epsilon)^{1/2}\cos(\theta/2)].\end{aligned} \tag{A3}$$

If we write Eq. (A1) as

$$P(f^{(2)},r,\theta)dr+Q(f^{(2)},r,\theta)d\theta-df^{(2)}=0 \tag{A4}$$

and define

$$\mathbf{Y}\triangleq[P,Q-1], \tag{A5}$$

then Eq. (A4) is integrable if and only if

$$\mathbf{Y}\cdot\operatorname{curl}\mathbf{Y}=0, \tag{A6}$$

(Ref. 8), i.e., if and only if

$$-P\frac{\partial Q}{\partial f^{(2)}}+Q\frac{\partial P}{\partial f^{(2)}}+\frac{\partial P}{\partial\theta}-\frac{\partial Q}{\partial r}=0. \tag{A7}$$

Direct substitution of the derivatives of P and Q in Eq. (A7) confirms Eq. (A6). □

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