Separation of variables on n-dimensional Riemannian manifolds. I. The n-sphere S_n and Euclidean n-space R_n

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The following problem is solved: What are all the "different" separable coordinate systems for the Laplace–Beltrami eigenvalue equation on the n-sphere S_n and Euclidean n-space R_n and how are they constructed? This is achieved through a combination of differential geometric and group theoretic methods. A graphical procedure for construction of these systems is developed that generalizes Vilenkin's construction of polyspherical coordinates. The significance of these results for exactly soluble dynamical systems on these manifolds is pointed out. The results are also of importance for the analysis of the special functions appearing in the separable solutions of the Laplace–Beltrami eigenvalue equation on these manifolds.

I. INTRODUCTION

In this paper we find all separable coordinate systems on the real n-sphere S_n and Euclidean n-space for the Hamilton–Jacobi equation

$$H = g^{ij}S_{x^i}S_{x^j} = E, \quad S_{x^i} = \frac{\partial S}{\partial x^i}, \quad i = 1,...,N, \tag{I}$$

and the Helmholtz equation

$$\Delta_n = \frac{1}{\sqrt{g}}\frac{\partial}{\partial x^i}\left(\sqrt{g}\,g^{ij}\frac{\partial \Psi}{\partial x^i}\right) = \lambda\Psi,$$
$$i,j = 1,...,n, \quad g = \det(g_{ij}). \tag{II}$$

There are several reasons why this is an important problem.

(1) The list of 11 coordinate systems in R_3 that provide a separation of variables for these equations are well known.[1] Their value in the solution of boundary value problems is unquestioned. More recently there has been an interest in separation of variables on the spheres S_2 and S_3 (see Refs. 2 and 3). In the case of S_3 the relationship with the hydrogen atom has been extensively studied.[4] More recently the importance of separable coordinate systems on S_n has been discussed[5] for dynamical symmetries in a spherical geometry. It is also of interest to study classical and quantum mechanics on S_n and R_n as a means for finding exactly soluble dynamical systems interacting under a suitable potential so as to admit solution via a separation of variables.

(2) On the mathematical side the solution of the problem we solve here gives the basic results necessary for a complete analysis of the special functions that are solutions of (II) via a separation of variables on S_m and R_n. In doing so all the separable solutions can be characterized in terms of symmetric second-order elements in the enveloping algebra of the corresponding symmetry group. This provides the basis for an all-embracing theory of such solutions and a systematic treatment of relations amongst these solutions. For an introduction to these methods we refer to Miller's book.[6] In solving this problem we also extend Vilenkin's work, which dealt with a restricted class of separable solutions.[7]

We should also note at this point the articles of Lucquaud,[8–10] which give a discussion of spherical harmonics on $SO(n)$ via an elegant tensorial approach. For some of the crucial results concerning separation of variables we refer the reader to the papers of Levi-Civita,[11] Eisenhart,[12] and Benenti.[13] Referring now to equations (I) and (II) we should, of course, mention that these equations are expressed in an arbitrary coordinate system in terms of which the infinitesmal distance on the underlying manifold is

$$ds^2 = g_{ij}\,dx^i\,dx^j, \quad i,j = 1,...,n. \tag{1.1}$$

[Formulas (I), (II), and (1.1) use the summation convection on indices i,j.] Separation of variables for (I) is understood to mean that there is a coordinate system $\{x^i\}$ for which it is possible to find a solution $S = S(\mathbf{x};\lambda_1,...,\lambda_n)$ of (I) such that

$$S = \sum_{i=1}^{n} S_i(x^i;\lambda_1,...,\lambda_n) \tag{1.2}$$

and $\det(\partial^2 S/\partial x^i\,\partial\lambda_j)_{n\times n} \neq 0$, i.e., S is a complete integral.[14] This type of variable separation is *additive*.

Separation of variables for (II) is normally understood in the product sense,[15] i.e., the coordinates $\{x^i\}$ should be such that there is a soluton of (II) depending on n parameters $c_1,...,c_n$ of the form

$$\Psi = \prod_{i=1}^{n} \Psi_i(x^i;c_1,...,c_n). \tag{1.3}$$

In this article we determine all coordinate systems that provide additive separation for (I) and product separation for (II) for the following Riemannian manifolds: (i) the real n-sphere S_n and (ii) real Euclidean n-space R_n. We also describe a graphical procedure for constructing these coordinates, which includes Vilenkin's description of polyspherical coordinates as a special case.

We recall a few basic facts about variable separation. For a positive definite Riemannian space a separable coordinate system $\{x^i\}$ for (I) can always be chosen[16,17] such that

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the contravariant metric tensor is

$$(g^{ij}) = \left[\begin{array}{c|c} \delta^{ab} H_a^{-2} & 0 \\ \hline 0 & g^{\alpha\beta} \end{array}\right]. \tag{1.4}$$

The functions H_a^{-2} and $g^{\alpha\beta}$ have the form

$$H_a^{-2} = \frac{\Phi^{a1}}{\Phi}, \quad g^{\alpha\beta} = \sum_b A_b^{\alpha\beta}(x^b) \frac{\Phi^{b1}}{\Phi}, \tag{1.5}$$

where $\Phi = \det(\Phi_{ab}(x^a))$. The variables x^α are such that $\partial g^{ij}/\partial x^\alpha = 0$, for all i, j.

A typical separable solution takes the form

$$S = \sum_a S_a(x^a) + \sum_\alpha c_\alpha x^\alpha.$$

The choice of ignorable variables x^α is not unique; we would get a similar system if we defined new coordinates $x^{\alpha'}$ by $x^{\alpha'} = a^\alpha_\beta x^\beta$, $x^{a'} = x^a$, where $\det(a^\alpha_\beta) \neq 0$. We say that two such coordinate systems are *equivalent* and will not distinguish between them.

The standard form (1.4) will be central to our arguments. If a coordinate system is separable for (II), it is automatically separable for (I). A separable system $\{x^i\}$ for (I) separates (II) if and only if

$$R_{ab} = 0, \quad a \neq b,$$

where R_{ij} is the Ricci tensor expressed in these coordinates. In particular, for orthogonal coordinates, (I) and (II) separate in the same systems.

A. The n-sphere S_n

This space is most readily realized in terms of $n+1$ real "standard" coordinates $(s_1,\ldots,s_{n+1}) \in R_{n+1}$, which satisfy

$$s_1^2 + \cdots + s_{n+1}^2 = 1. \tag{1.6}$$

The infinitesimal distance is given by

$$ds^2 = ds_1^2 + \cdots + ds_{n+1}^2. \tag{1.7}$$

The n-sphere admits the group $\mathrm{SO}(n+1)$ of isometries. The algebra $\mathrm{so}(n+1)$ is realized on the cotangent bundle of R_{n+1} by the Killing vectors

$$I_{ij} = s_i p_{s_j} - s_j p_{s_i}, \quad i \neq j. \tag{1.8}$$

We recall in the normal correspondence, $\partial S/\partial x^i = p_i$ and L is a Killing vector if L is linear in the p_i's and $\{H,L\} = 0$ where $\{\ ,\ \}$ is the Poisson bracket. It is then seen that the ignorable coordinates x^α of a given separable coordinate system are such that p_α is a Killing vector. The Lie algebra $\mathrm{so}(n+1)$ also can be realized by means of linear differential operators, with the identification $p_{s_i} \to \partial/\partial s_i$. The symmetry operator $\hat{I}_{ij} = s_i(\partial/\partial s_j - s_j \partial/\partial s_i)$ satisfies $[\Delta_n, \hat{I}_{ij}] = 0$, where $[\ ,\ ]$ is the commutator bracket and Δ_n is the operator (II) on S_n. We note that the two realizations of $\mathrm{so}(n+1)$ directly relate to the $\mathrm{SO}(n+1)$-invariant equations (I) and (II). For equation (I) the algebra is realized as the set of all Killing vectors L that are in involution with H, i.e., $\{H,L\} = 0$. For equation (II) the algebra is realized by all first-order linear differential operators $\mathscr{L}$ that commute with Δ_n. The n-sphere as a Riemannian manifold is a space of constant curvature -1 and is completely characterized by the Riemann curvature tensor conditions[18]

$$R_{hijk} = (g_{hk} g_{ij} - g_{hj} g_{ik}), \tag{1.9}$$

in any coordinate system.

B. Euclidean n-space R_n

Here, a point is given by n real (Cartesian) coordinates $(y_1,\ldots,y_n)$ and the infinitesimal distance is

$$ds^2 = dy_1^2 + \cdots + dy_n^2, \tag{1.10}$$

where R_n admits the isometry group $E(n) = T_n \otimes \mathrm{SO}(n)$. This is the semidirect product of the n-dimensional Abelian group of translations T_n and $\mathrm{SO}(n)$. On the cotangent bundle of R_n the Lie algebra $\mathscr{E}(n)$ has a realization by Killing vectors:

$$M_{ij} = y_i p_{y_j} - y_j p_{y_i}, \quad P_k = p_{y_k}, \quad i,j,k = 1,\ldots,n, \quad i \neq j. \tag{1.11}$$

The corresponding realization in terms of symmetry operators can be obtained by the correspondence $p_j \to \partial/\partial y_j$. Euclidean n-space is characterized by the Riemann curvature tensor condition $R_{hijk} \equiv 0$ in any coordinate system.

We note that the study of variable separation will give a complete enumeration of the scope and extent of special function identities available in these spaces. In addition, exactly which special functions appear can be determined. The problem of separation of variables on S_n is also intimately related to the separation of variables problem on $\mathrm{CP}(n)$,[19] n-dimensional complex projective space.

II. SEPARATION OF VARIABLES ON S_n

The following is a crucial result in the classification of separable coordinate systems on S_n.

Theorem: Let $\{x^i\}$ be a coordinate system on S_n for which the Hamilton–Jacobi equation admits a separation of variables. Then, by passing to an equivalent system of coordinates if necessary, we have $g^{ij} = \delta^{ij} H_i^{-2}$, i.e., separation of variables occurs only in orthogonal coordinates. Furthermore, in terms of the standard coordinates on the sphere $s_1,\ldots,s_{n+1}$, the ignorable variables can be chosen such that

$$p_{\alpha_1} = I_{12}, \quad p_{\alpha_2} = I_{34}, \ldots, p_{\alpha_q} = I_{2q+1,2q+2}. \tag{2.1}$$

where the number of ignorable variables is q.

Proof: This is based on the general block-diagonal expression of the canonical form of the contravariant metric tensor for a separable coordinate system. It is well known[20] that any element of the symmetry algebra $\mathrm{so}(n+1)$ of S_n is conjugate to an element of the form

$$L = I_{12} + b_2 I_{34} + \cdots + b_\nu I_{2\nu-1,2\nu}. \tag{2.2}$$

If this element corresponds to the ignorable variable α_1, i.e., $L = p_{\alpha_1}$, then by local Lie theory the standard coordinates on the n-sphere can be taken as

$$(s_1,\ldots,s_{n+1}) = (\rho_1 \cos(\alpha_1 + w_1), \rho_1 \sin(\alpha_1 + w_1), \rho_2 \cos(b_2\alpha_1 + w_2), \rho_2 \sin(b_2\alpha_1 + w_2), \ldots, \rho_\nu \cos(b_\nu\alpha_1 + w_\nu), \rho_\nu \sin(b_\nu\alpha_1 + w_\nu), s_{2\nu+1},\ldots,s_{n+1}), \tag{2.3}$$

where $\rho_1^2 + \cdots + \rho_\nu^2 + s_{2\nu+1}^2 + \cdots + s_{n+1}^2 = 1$. The infinitesimal distance then has the form

$$ds^2 = d\rho_1^2 + \cdots + d\rho_\nu^2 + \rho_1^2(d\alpha_1 + dw_1)^2 + \cdots + \rho_\nu^2(b_\nu\, d\alpha_1 + dw_\nu)^2 + ds_{2\nu+1}^2 + \cdots + ds_{n+1}^2. \tag{2.4}$$

If there is only one ignorable variable then the coordinate system must be orthogonal and this is only possible if $b_2 = \cdots = b_\nu = 0$, i.e., $p_{\alpha_1} = I_{12}$. Indeed, the requirement that the contravariant metric have the form (1.4) (orthogonal in this case) is that

$$-dw_1 = \sum_{j=2}^{\nu} \frac{\rho_j^2}{\rho_1^2} b_j\, dw_j. \tag{2.5}$$

Since the differentials $d\rho_j, dw_j$ ($j \geqslant 2$), must be independent and the only condition on ρ_1^2 is

$$\sum_{i=1}^{\upsilon} \rho_i^2 + s_{2\upsilon+1}^2 + \cdots + s_{n+1}^2 = 1,$$

the condition $dw_1^2 = 0$ implies $b_j = 0, j = 2,...,\nu$, and $dw_1 = 0$. We can then take the constant $w_1 = 0$ by suitably redefining α_1. The theorem is proven in this case.

Now suppose there are $q > 1$ ignorable variables. The Killing vectors p_{α_i}, $i = 1,...,q$, must form an involutive set. It follows from the spectral theorem for commuting skew-adjoint matrices that for each i, p_{α_i} has a representation of the form

$$p_{\alpha_i} = b_1^i I_{12} + b_2^i I_{34} + \cdots + b_{\nu_i}^i I_{2\nu_i - 1,2\nu_i}, \tag{2.6}$$

for $i = 2,..,q$. In fact we can assume

$$p_{\alpha_i} = I_{2i-1,2i} + \sum_{l>q}^{N} b_l^i I_{2l-1,2l}, \quad i = 1,...,q. \tag{2.7}$$

The projective coordinates on the sphere then have the form

$$\begin{aligned}(s_1,...,s_{n+1}) = \Big(&\rho_1 \cos(\alpha_1 + w_1), \rho_1 \sin(\alpha_1 + w_1),...,\rho_q \cos(\alpha_q + w_q), \rho_q \sin(\alpha_q + w_q),\\ &\rho_{q+1} \cos\Big(\sum_{i=1}^{q} b_{q+1}^i \alpha_i + w_{q+1}\Big),\ \rho_{q+1} \sin\Big(\sum_{i=1}^{q} b_{q+1}^i \alpha_i + w_{q+1}\Big),...,\\ &\rho_N \sin\Big(\sum_{i=1}^{q} b_N^i \alpha_i + w_N\Big), s_{2N+1},...,s_{n+1}\Big).\end{aligned} \tag{2.8}$$

We now make the crucial requirement that the ignorable variables α_i, $i = 1,...,q$, are part of a separable coordinate system. If we compute the covariant metric, it should be in block-diagonal form with respect to the two classes of variables. Just as in the case $q = 1$, this is only possible if $b_l^i = 0$, $i = 1,..,q$, $l = q+1,...,N$ and $dw_i = 0$, $1 < i \leqslant q$. We can therefore assume that $L_1 = I_{12}, L_2 = I_{34},...,L_q = I_{2q-1,2q}$; the ignorable coordinates α_i then can always be chosen such that $w_i = 0$, $1 < i \leqslant q$, and the system is orthogonal. Q.E.D.

This theorem enables us to bring to bear Eisenhart's[12] results on orthogonal systems of the Stäckel type. Our problem reduces to the enumeration of all orthogonal separable coordinate systems. We use an inductive procedure such that given all separable systems for $S_j, j < n$, we can give the rules for construction of all systems on S_n.

If $\{x^i\}$ is an orthogonal coordinate system with infinitesimal distance $ds^2 = \Sigma_{i=1}^n H_i^2 (dx^i)^2$, then the conditions that the space be of constant curvature -1, i.e., that we are dealing with S_n, are

$$\begin{aligned}&\text{(i)} \quad R_{ijji} = -H_i^2 H_j^2, \quad i \neq j,\\ &\text{(ii)} \quad R_{hiik} = 0, \quad i \neq h \neq k.\end{aligned} \tag{2.9}$$

Eisenhart[12] showed that in order for orthogonal separation to occur on any n-dimensional Riemannian manifold the contravariant metric $g^{ij} = \delta^{ij} H_i^{-2}$ must be in Stäckel form and that the necessary and sufficient conditions for this are

$$\frac{\partial^2}{\partial x^j \partial x^k} \log H_i^2 - \frac{\partial}{\partial x^j} \log H_i^2 \frac{\partial}{\partial x^k} \log H_i^2 + \frac{\partial}{\partial x_j} \log H_i^2 \frac{\partial}{\partial x_k} \log H_j^2 + \frac{\partial}{\partial x_k} \log H_i^2 \frac{\partial}{\partial x_j} \log H_k^2 = 0, \tag{2.10}$$

for $j \neq k$. He then went further to show that these conditions, together with the equations (2.9) (ii), are equivalent to the equations

$$\frac{\partial}{\partial x^j} \log H_i^2 \frac{\partial}{\partial x^k} \log H_i^2 - \frac{\partial}{\partial x^j} \log H_i^2 \frac{\partial}{\partial x^k} \log H_j^2 - \frac{\partial}{\partial x^k} \log H_i^2 \frac{\partial}{\partial x^j} \log H_k^2 = 0, \quad i,j,k \text{ pairwise distinct.} \tag{2.11}$$

It follows that the metric for a separable system can be written in the form

$$g_{ii} = H_i^2 = X_i \prod_{j \neq i} (\sigma_{ij} + \sigma_{ji}), \quad i = 1,...,n, \tag{2.12}$$

where X_i, σ_{ij} are functions of x^i at most. The conditions (2.9) (i) are then equivalent to

$$\sigma_{ji}' \sigma_{ki}' (\sigma_{jk} + \sigma_{kj}) - \sigma_{ji}' \sigma_{kj}' (\sigma_{ki} + \sigma_{ik}) - \sigma_{ki}' \sigma_{jk}' (\sigma_{ij} + \sigma_{ji}) = 0, \quad i,j,k \text{ distinct}, \tag{2.13}$$

where $\sigma'_{kl} = (\partial_x k)\sigma_{kl}$, etc. We now study various possibilities for the functions σ_{ij}. If all the functions σ_{ij} are such that $\sigma'_{ij} \neq 0$ then Eisenhart has shown that the metric coefficients have the form

$$g_{ii} = H_i^2 = X_i \prod_{j \neq i} (\sigma_i - \sigma_j), \tag{2.14}$$

where $\sigma_i = \sigma_i(x^i)$ and $\sigma'_i \neq 0$. This metric will be the basic building block on which we can formulate our inductive construction. Without loss of generality we can redefine variables $\{x^i\}$ in such a way that $\sigma_i = x^i$, i.e.,

$$H_i^2 = X_i \prod_{j \neq i} (x^i - x^j). \tag{2.15}$$

The conditions (2.9) (i) then amount to

$$\left[\prod_{l \neq j} (x^j - x^l)\right]^{-1} \left\{\frac{-2}{(x^i - x^j)^2}\left(\frac{1}{X_j}\right) + \frac{-1}{(x^i - x^j)}\left(\frac{1}{X_j}\right)'\right\} + \left[\prod_{l \neq i} (x^i - x^l)\right]^{-1} \left\{\frac{-2}{(x^i - x^j)^2}\left(\frac{1}{X_i}\right) + \frac{-1}{(x^j - x^i)}\left(\frac{1}{X_i}\right)'\right\}$$
$$+ \sum_{l \neq i,j} \frac{1}{X_l (x^l - x^i)(x^l - x^j) \prod_{k \neq l} (x^l - x^k)} = -4. \tag{2.16}$$

These equations have the solution

$$(1/X_i)^{(n+1)} + 4(n+1)! = 0, \quad i = 1,...,n. \tag{2.17}$$

i.e.,

$$\frac{1}{X_i} = -4(x^i)^{n+1} + \sum_{l=0}^{n} a_l (x^i)^{n-l} = f(x^i).$$

The function $f(x)$ can also be written

$$f(x) = -4 \prod_{i=1}^{n+1} (x - e_j). \tag{2.18}$$

There are two requirements to determine which metrics of this type occur on S_n: (1) the metric must be positive definite and (2) the variables x^i should vary in such a way that they correspond to a coordinate patch that is compact. There is a unique solution to these requirements: the x^i, e_i should satisfy

$$e_1 < x^1 < e_2 < \cdots < e_n < x^n < e_{n+1}. \tag{2.19}$$

These are elliptic coordinates on the n-sphere S_n. They can be related to the coordinates $\{s_j\}$ via

$$s_j^2 = \frac{\prod_{i=1}^{n} (x^i - e_j)}{\prod_{j \neq i} (e_i - e_j)}, \quad j = 1,...,n+1. \tag{2.20}$$

These systems are the basic building blocks for separable coordinate systems on real spheres. To complete the analysis of possible orthogonal separable systems we need to consider the case when some of the σ_{ij} functions are constants. If $\sigma_{ij} = a_{ij}$ (const), Eisenhart has shown that there are four possibilities:

(i) $\sigma_{ij} = a_{ij}$, $\sigma_{ji} = a_{ji}$,
$\sigma_{ik} = a_{ik}$, $\sigma_{jk} = a_{jk}$;

(ii) $\sigma_{ij} = a_{ij}$, $\sigma_{ji} = a_{ji}$,
$\sigma_{ik} = a_{ik}$, $\sigma_{ki} = a_{ki}$;

(iii) $\sigma_{ij} = a_{ij}$, $\sigma_{ik} = a_{ik}$,
$\sigma_{ji} = a_{ji}\sigma_j$, $\sigma_{jk} = a_{jk}\sigma_j$,
$\sigma_{ki} = a_{ki}\sigma_k$, $\sigma_{kj} = a_{kj}\sigma_k$;

(iv) $\sigma_{ij} = a_{ij}$, $\sigma_{kj} = a_{kj}$,
$\sigma_{ji} = a_{ji}\sigma_j$, $\sigma_{jk} = a_{jk}\sigma_j$,
$a_{ji}a_{kj} - a_{jk}a_{ij} = 0$; (2.21)

where σ_j is a function of x^j only and i,j,k are pairwise distinct. If we fix i and j, then, for k values corresponding to cases (i)–(iii), $\sigma_{ik} = a_{ik}$. To examine how the inductive process works let us take $\sigma_{1l} = a_{1l}$ for $l = k+1,...,n$ and $\sigma'_{1j} \neq 0$ for $j = 2,...,k$. Then we have

$$\sigma_{jl} = a_{jl}, \quad \sigma_{l1} = a_{l1}\sigma_l, \quad \sigma_{lj} = a_{lj}\sigma_l,$$
$$a_{l1}a_{jl} - a_{lj}a_{1l} = 0, \quad \text{for } l = k+1,...,n, \quad j = 2,...,k.$$

Assuming that $a_{lj} \neq 0$ for $l = k+1,...,n$, $j = 2,...,k$, we find the metric coefficients have the form

$$H_i^2 = \left[X_i \prod_{j \neq i} (\sigma_{ij} + \sigma_{ji})\right]\left[\prod_{l=k+1}^{n} (a_{il} + a_{li}\sigma_l)\right], \quad i = 1,...,k, \tag{2.22}$$

$$H_l^2 = X_l \prod_{\substack{1<j<k \\ m \neq l \\ m > k+1}} (\sigma_{lm} + \sigma_{ml}), \quad l = k+1,...,n. \tag{2.23}$$

Let us assume that no further functions σ_{ij}, σ_{lm} are constants. Then using the results of Eisenhart we can take the metric coefficients as

$$H_i^2 = \left[X_i \prod_{j \neq i} (x^i - x^j)\right]\left(\prod_{l=k+1}^{n} \sigma_l\right),$$
$$H_l^2 = \left[X_l \prod_{m \neq l} (x^l - x^m)\right]. \tag{2.24}$$

The conditions $R_{klik} = -H_k^2 H_l^2$ are equivalent to (2.16) and (2.17) with $i = k+1,...,n$ and $n \to k = n'$. Putting

$$H_i^2 = \left[X_i \prod_{j \neq i} (x^i - x^j)\right],$$

the conditions $R_{ijji} = H_i^2 H_j^2$ and $R_{illi} = -H_i^2 H_l^2$ are equivalent to

$$H_i^{-2} H_j^{-2} R_{ijji} + \left(\prod_{l=k+1}^{n} \sigma_l\right) \times \left[\sum_{l'=k+1}^{n} \frac{1}{4H_{l'}^2}\left(\frac{\sigma'_l}{\sigma_l}\right)^2 + 1\right] = 0, \tag{2.25}$$

$$2\frac{\sigma_l''}{\sigma_l}-\left(\frac{\sigma_l'}{\sigma_l}\right)^2-\left(\frac{\sigma_l'}{\sigma_l}\right)\times\left[\frac{\partial}{\partial x^l}\log H_l^2+H_l^2\sum_{m\neq l}\frac{1}{H_m^2(x^l-x^m)}\right]=-4H_l^2, \tag{2.26}$$

where $\tilde{R}_{ijji}$ is the Riemann curvature tensor for the Riemannian manifold with infinitesimal distance $ds^2=\sum_{i=1}^k \tilde{H}_i^2(dx^i)^2$. These equations are satisfied if and only if

$$\frac{1}{X_l}=-4\prod_{m=1}^{n-k+1}(x^l-f_m),\quad l=k+1,\ldots,n, \tag{2.27}$$

and $\sigma_l=(x^l-f_{n-k+1})/(f_{l-k}-f_{n-k+1})$, where we take $f_1<f_2<\cdots<f_{n-k+1}$. The remaining condition then is $\tilde{R}_{ijji}=-\tilde{H}_i^2\tilde{H}_j^2$ so that

$$\frac{1}{X_i}=-4\prod_{j=1}^{k+1}(x^i-e_j). \tag{2.28}$$

The coordinates on S_n can be taken as

$$(s_1,\ldots,s_{n+1})=(u_1v_1,\ldots,u_1v_{k+1},u_2,\ldots,u_{n-k+1}), \tag{2.29}$$

where

$$\sum_{i=1}^{k+1}v_i^2=1,\qquad \sum_{l=1}^{n-k+1}u_l^2=1,$$

and

$$v_j^2=-\frac{\Pi_{i=1}^k(x^i-f_j)}{\Pi_{j\neq i}(f_i-f_j)}, \tag{2.30}$$

$$u_m^2=-\frac{\Pi_{l=k+1}^n(x^l-e_m)}{\Pi_{n\neq m}(e_n-e_m)}. \tag{2.31}$$

The infinitesimal distance has the form

$$ds_0^2=ds_1^2\left[\frac{\Pi_{l=k+1}^n(x^l-f_{n-k+1})}{\Pi_{m\neq n-k+1}(f_m-f_{n-k+1})}\right]+ds_2^2, \tag{2.32}$$

where

$$ds_1^2=-\frac{1}{4}\sum_{i=1}^k\left[\frac{\Pi_{j\neq i}(x^i-x^j)}{\Pi_{j=1}^{k+1}(x^i-e_j)}\right](dx^i)^2, \tag{2.33}$$

$$ds_2^2=\frac{-1}{4}\sum_{l=k+1}^n\left[\frac{\Pi_{m\neq l}(x^l-x^j)}{\Pi_{m=1}^{n+k+1}(x^l-f_m)}\right](dx^l)^2,\qquad m=k+1,\ldots,n,\quad j=1,\ldots,k. \tag{2.34}$$

The choice of embedding of the sphere S_k in the n-sphere S_n given by (2.29) is not, of course, unique. It is here we meet the second concept involved in regarding two choices of coordinates $(s_1,\ldots,s_{n+1})$ as giving "equivalent" coordinate systems. Clearly we could subject the coordinates $\{s_i\}$ to an arbitrary $SO(n+1)$ group action. The infinitesimal distance would remain unchanged in the process. We regard the new set of coordinates $(s_1',\ldots,s_{n+1}')$ as equivalent to the original set. This is just the mathematical formulation of the geometric identification of coordinate systems that differ only by an isometry. This aspect of equivalence is obviously group related. If the Riemannian manifold had no isometry group it would not be relevant.

Now suppose one of the constants $a_{ij}=0$ for some fixed l and j. Then from the relations

$$a_{l1}a_{jl}-a_{lj}a_{1l}=0, \tag{2.35}$$

we have $a_{l1}=0$ and consequently $a_{li}=0$, for $i=1,\ldots,k$. This implies that σ_l does not appear in H_i^2, $i=1,\ldots,k$.

Referring to the curvature equation $R_{illi}=-H_i^2H_l^2$ we see that it cannot be satisfied if $\sigma_{li}=a_{li}\sigma_l=0$ as this would imply $-4H_l^2=0$. Thus $a_{ij}\neq 0$ for each l,j. Recall here that we have assumed that none of the functions σ_{ij} $(i,j=1,\ldots,k,\ i\neq j)$, σ_{lm} $(l,m=k+1,\ldots,n,\ l\neq m)$ is a constant. Let us now push this process one step further: Let $\sigma_{k+1,s}=a_{k+1,s}$ for $s=p+1,\ldots,n$ and $\sigma_{k+1,s}'\neq 0$ for $s=k+1,\ldots,p$. Then applying the same arguments as previously, we see that the metric coefficients H_l^2, $l=k+1,\ldots,n$, can be brought to the form

$$H_l^2=X_l\left[\prod_{\substack{m\neq l\\ k+1<l<p}}(\sigma_{lm}+\sigma_{ml})\right]\left[\prod_{s=p+1}^n(a_{ls}+a_{sl}\sigma_s)\right], \tag{2.36}$$

$$H_t^2=X_t\left[\prod_{\substack{s\neq t\\ s>p+1}}(\sigma_{st}+\sigma_{ts})\right]. \tag{2.37}$$

Here the indices run over the ranges

$$i,j,\ldots=1,\ldots,k,\quad l,m,\ldots=k+1,\ldots,p,\quad s,t,u,\ldots=p+1,\ldots,n. \tag{2.38}$$

We follow this convention unless otherwise stated. If none of the remaining σ_{ab}'s are constants there are two cases to consider:

(i) $a_{ls}/a_{sl}=a_{is}/a_{si}$,

for $s=p+1,\ldots,n,\quad i=1,\ldots,k,\quad l=k+1,\ldots,p$.

Then the infinitesimal distance has the form

$$ds^2=\left(\prod_{t=p+1}^n\sigma_t\right)d\omega^2+\sum_{t=p+1}^n X_t\left[\prod_{u\neq t}(\sigma_{ut}+\sigma_{tu})\right](dx^t)^2, \tag{2.39}$$

where

$$d\omega^2=\left(\prod_{l=k+1}^p\sigma_l\right)\sum_{i=1}^k X_i\left[\prod_{j\neq i}(\sigma_{ij}+\sigma_{ji})\right](dx^i)^2+\sum_{l=k+1}^p X_l\left[\prod_{m\neq l}(\sigma_{lm}+\sigma_{ml})\right](dx^l)^2. \tag{2.40}$$

The form $d\omega^2$ corresponds to the choice of metric coefficients with $l=k+1,\ldots,p<n$. If we impose the conditions $R_{abba}=-H_a^2H_b^2$, then we see that for $a,b=1,\ldots,k,k+1,\ldots,p$ the conditions are identical with (2.16). Hence

$$\frac{1}{X_i}=-4\prod_{j=1}^{k+1}(x^i-e_j),\quad i=1,\ldots,k, \tag{2.41}$$

$$\frac{1}{X_l}=-4\prod_{m=1}^{p-k+1}(x^l-f_m),\quad l=k+1,\ldots,p, \tag{2.42}$$

and

$$\sigma_l=\frac{(x^l-f_{p-k+1})}{(f_{l-k}-f_{p-k+1})},\quad l=k+1,\ldots,p. \tag{2.43}$$

The remaining conditions

$$R_{tuut} = -H_t^2 H_u^2$$

and

$$R_{taat} = -H_a^2 H_t^2 \ (a = 1,...,p)$$

also imply

$$\frac{1}{X_s} = -4 \prod_{t=1}^{n-p+1} (x^s - g_t), \quad s = p+1,...,n, \tag{2.44}$$

and

$$\sigma_t = \frac{(x^t - g_{n-p+1})}{(g_{t-p} - g_{n-p+1})}, \quad t = p+1,...,n.$$

These coordinates on S_n can then be constructed in a standard way:

$$(s_1,...,s_{n+1}) = (u_1v_1w_1,...,u_1v_1w_{k+1},u_1v_2,...,u_1v_{p-k+1},u_2,...,u_{n-p+1}), \tag{2.45}$$

where

$$\sum_{i=1}^{k+1} w_i^2 = 1, \quad \sum_{l=1}^{p-k+1} v_l^2 = 1, \quad \sum_{i=1}^{n-p+1} u_i^2 = 1,$$

and on each of the spheres defined by the u_i, v_j, and w_k coordinates, elliptic coordinates are chosen, i.e.,

$$v_j^2 = \frac{-\Pi_{q=1}^{k}(x^q - e_j)}{\Pi_{j\neq i}^{k+1}(e_i - e_j)}, \quad j,i = 1,...,k+1, \tag{2.46}$$

$$w_l^2 = \frac{-\Pi_{q=k+1}^{p}(x^q - f_l)}{\Pi_{m\neq l}(f_m - f_l)}, \quad m,l = 1,...,p-k+1, \tag{2.47}$$

$$u_t^2 = \frac{-\Pi_{q=p+1}^{n}(x^q - g_t)}{\Pi_{s\neq t}(g_s - g_t)}, \quad s,t = 1,...,n-p+1. \tag{2.48}$$

Now

(ii) $a_{ls}/a_{sl} \neq a_{is}/a_{si}$.

In this case $\sigma_l = a_l$, for $l = k+1,...,p$, as follows from Eisenhart's cases (2.21) (i)–(2.21)(iv). The infinitesimal distance has the form

$$ds^2 = \left(\prod_{t=p+1}^{n} \sigma_t\right) d\omega_1^2 + \left(\prod_{t=p+1}^{n} (\sigma_t + \alpha)\right) d\omega_2^2 + \sum_{t=p+1}^{n} X_t \left[\prod_{\substack{u\neq t \\ u>p+1}} (\sigma_{ut} + \sigma_{tu})\right] (dx^t)^2, \quad \alpha \neq 0, \tag{2.49}$$

where

$$d\omega_1^2 = \sum_{i=1}^{k} X_i \left[\prod_{\substack{j\neq i \\ j<k}} (\sigma_{ij} + \sigma_{ji})\right] (dx^i)^2, \tag{2.50}$$

$$d\omega_2^2 = \sum_{l=k+1}^{p} X_l \left[\prod_{\substack{m\neq l \\ k+1<m<p}} (\sigma_{lm} + \sigma_{ml})\right] (dx^l)^2. \tag{2.51}$$

The conditions that this metric correspond to S_n require that we have the same functions X_a as in the previous case and now

$$\sigma_t = \frac{(x^t - g_1)}{(g_{t-p+1} - g_1)}, \quad \sigma_t + \alpha = \frac{(x^t - g_2)}{(g_{t-p+2} - g_2)}. \tag{2.52}$$

Here we have adopted the convention

$$g_{n-p+1+l} = g_l, \quad \text{for } k+1 \leqslant l \leqslant p. \tag{2.53}$$

Consequently the infinitesimal distance has the form

$$ds^2 = \left[\frac{\Pi_{t=p+1}^{n}(x^t - g_1)}{\Pi_{u\neq t}(g_u - g_1)}\right] d\omega_1^2 + \left[\frac{\Pi_{t=p+1}^{n}(x^t - g_2)}{\Pi_{u\neq t}(g_u - g_2)}\right] d\omega_2^2 - \frac{1}{4} \sum_{t=p+1}^{n} \left[\frac{\Pi_{u\neq t,\, p+1\leqslant u\leqslant n}(x^t - x^u)}{\Pi_{u=p+1}^{n+1}(x^t - g_u)}\right] (dx^t)^2. \tag{2.54}$$

A standard choice of coordinates on S_n for this infinitesimal distance can be taken as

$$(s_1,...,s_{n+1}) = (u_1v_1,...,u_1v_{k+1},u_2w_1,...,u_2w_{p+1},u_3,...,u_{n-p-k-1}), \tag{2.55}$$

with u_i, v_j, and w_k coordinates as in (2.45). This procedure can be iterated without difficulty to find all separable coordinate systems on S_n. If we do this we obtain an infinitesimal distance of the form

$$ds^2 = \sum_{I=1}^{p} \left\{\sum_{i\in N_I} (H_i^I)^2 (dx^i)^2\right\} \left[\prod_{l\in N_{p+1}} (\sigma_l + \alpha_I)\right] + \sum_{j\in N_{p+1}} (H_j^{p+1})^2 (dx^j)^2, \quad \alpha_I \neq \alpha_J, \quad \text{if } I \neq J. \tag{2.56}$$

Here $\{N_1,...,N_{p+1}\}$ is a partition of the integers $1,...,n$ into mutually exclusive sets N_I, i.e., $N_I \cap N_J = \varnothing$. It follows from Eisenhart's types (2.21) (i)–(2.21) (iv) that $(\partial_{x^j}) H_i^{(I)} = 0$ if $j \notin N_I$. The curvature conditions can now be written down. The conditions $R_{ijji} = -H_i^2 H_j^2$ $(i \neq j)$ are equivalent to the equations

$$R_{ijji}^{(p+1)} = -(H_i^{p+1})^2 (H_u^{p+1})^2, \quad i,j \in N_{p+1}, \tag{2.57}$$

$$(H_i^I)^{-2}(H_j^I)^{-2} R_{ijji}^{(I)} + \left[\prod_{K\in N_{p+1}} (\sigma_k + \alpha_I)\right] \times \left[\frac{1}{4} \sum_{k\in N_{p+1}} (H_l^{(p+1)})^{-2} \frac{\sigma_l'^2}{(\sigma_l + \alpha_I)^2} + 1\right] = 0, \quad i,j \in N_I, \tag{2.58}$$

$$2\frac{\sigma_l''}{(\sigma_l + \alpha_I)} - \left(\frac{\sigma_l'}{\sigma_l + \alpha_I}\right)^2 - \left(\frac{\sigma_l'}{(\sigma_l + \alpha_I)}\right) \left[\frac{\partial}{\partial x^l} \log (H_l^{(p+1)})^2 + (H_l^{(p+1)})^2 \sum_{\substack{m\neq l \\ m\in N_{p+1}}} \frac{1}{(H_m^{(p+1)})^2 (x^l - x^m)}\right] = -4(H_l^{(p+1)})^2, \quad l \in N_{p+1}, \tag{2.59}$$

$$\frac{1}{4}\sum_{l\in N_{p+1}}\frac{1}{(H_l^{(p+1)})^2}\frac{\sigma_l'^2}{(\sigma_l+\alpha_I)(\sigma_l+\alpha_J)}=-1. \tag{2.60}$$

Here we have used the notation $R^{(I)}_{hijk}$ to refer to the curvature tensor of the Riemannian manifold with infinitesimal distance

$$d\omega_I^2=\sum_{l\in N_I}(H_l^{(I)})^2(dx^l)^2. \tag{2.61}$$

These equations have the solutions

$$\left[\prod_{l\in N_{p+1}}(\sigma_l+\alpha_I)\right]=\frac{\Pi_{l\in N_{p+1}}(x^l-e_I)}{\Pi_{m\in N_{p+1}}(e_m-e_I)}, \tag{2.62}$$

$$(H_l^{p+1})^2=\frac{-1}{4}\left[\frac{\Pi_{m\in N_{p+1}(m\neq l)}(x^m-x^l)}{\Pi_{n=1}^{n_{p+1}+1}(x^l-e_n)}\right],\quad l\in N_{p+1}, \tag{2.63}$$

$$R^{(I)}_{ijji}=-(H_i^{(I)})^2(H_j^{(I)})^2,$$
$$I=1,...,p+1,\quad i,j\in N_I, \tag{2.64}$$

where $n_{p+1}=\dim N_{p+1}$. The infinitesimal distance can always be written in the form

$$ds^2=\sum_{I=1}^{p}d\omega_I^2\left[\frac{\Pi_{l=1}^{n_1}(x^l-e_I)}{\Pi_{m\neq I}(e_m-e_I)}\right]$$
$$-\frac{1}{4}\sum_{i=1}^{n_1}\left[\frac{\Pi_{j=1}(x^i-x^j)}{\Pi_{j=1}^{n_1+1}(x^i-e_j)}\right](dx^i)^2, \tag{2.65}$$

where each $d\omega_I^2$ is the infinitesimal distance of a S_{p_a}. The coordinates on each S_{p_a} are again separable. Clearly we must have the constraint $\Sigma_{I=1}^{p}p_I+n_1=n$. Using this infinitesimal distance we can construct all separable coordinate systems inductively. The basic building blocks of separable coordinate systems are the elliptic coordinates on spheres of various dimensions. We will prescribe a graphical procedure for obtaining admissible coordinate systems, essentially giving the admissible embeddings of spheres inside spheres, which are allowed so as to correspond to separable coordinates.

III. THE CONSTRUCTION OF SEPARABLE COORDINATE SYSTEMS ON S_n

As we have seen in the previous section the basic building blocks of separable coordinate systems on S_n are the p-sphere elliptic coordinates

$${}_ps_j^2=\frac{\Pi_{l=1}^{p}(x^l-e_j)}{\Pi_{j\neq i}(e_i-e_j)},\quad \sum_{j=1}^{p+1}{}_ps_j^2=1,$$
$$p=1,...,n,\quad j=1,...,p+1. \tag{3.1}$$

Two important examples of these coordinates are

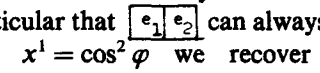
$$\text{(i)}\quad p=1:\quad {}_1s_1^2=\frac{(x^1-e_1)}{(e_2-e_1)},\quad {}_1s_2^2=\frac{(x^1-e_2)}{(e_1-e_2)}, \tag{3.2}$$

where ${}_1s_1^2+{}_1s_2^2=1$, $e_1<x^1<e_2$; and

$$\text{(ii)}\quad p=2:\quad {}_2s_1^2=\frac{(x^1-e_1)(x^2-e_1)}{(e_2-e_1)(e_3-e_1)},$$
$${}_2s_2^2=-\frac{(x^1-e_2)(x^2-e_2)}{(e_2-e_1)(e_3-e_1)},$$
$${}_2s_3^2=\frac{(x^1-e_3)(x^2-e_3)}{(e_3-e_1)(e_3-e_2)}, \tag{3.3}$$

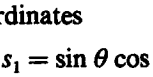
where ${}_2s_1^2+{}_2s_2^2+{}_2s_3^2=1$, $e_1<x^1<e_2<x^2<e_3$.

We will develop a graphical calculus for calculating admissible coordinate systems. We represent elliptical coordinates on S_n by the "irreducible" block



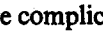
. (3.4)

Each separable coordinate system will be associated with a directed tree graph. Consider, for example, the sphere S_2. There are two possibilities.

(1) The first possibility is the irreducible block 

. Most treatments of elliptic coordinates on S_2 correspond to the choice $e_1=0, e_2=1, e_3=a>1$. This is just a reflection of the fact that for Jacobi elliptic coordinates the variables x^i and e_i always can be subjected to the transformation

$$x^{i'}=ax^i+b,\quad e_j'=ae_j+b,$$
$$i=1,...,n,\quad j=1,...,n+1. \tag{3.5}$$

Thus we can always choose $e_1=0$ and $e_2=1$. [Note in particular that 

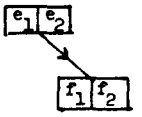
can always be replaced by 

. Putting $x^1=\cos^2\varphi$ we recover ${}_1s_1=\cos\varphi$, ${}_1s_2=\sin\varphi$ $(0<\varphi<2\pi)$.]

(ii) The second system is the usual choice of spherical coordinates

$$s_1=\sin\theta\cos\varphi,\quad s_2=\sin\theta\sin\varphi,\quad s_3=\cos\theta. \tag{3.6}$$

This system can be considered as the result of attaching a circle to a circle and is the prototype for the construction of more complicated systems. The graph

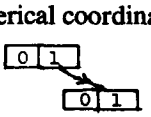


(3.7)

is taken to correspond to the choice of coordinates

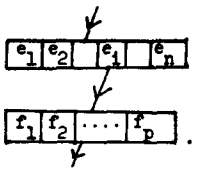
$$s_1^2={}_1u_1^2=\frac{(x^1-e_1)}{(e_2-e_1)},$$
$$s_2^2=({}_1u_2^2)({}_1v_1^2)=\frac{(x^1-e_2)}{(e_1-e_2)}\frac{(x^2-f_1)}{(f_2-f_1)}, \tag{3.8}$$
$$s_3^2=({}_1u_2^2)({}_1v_2^2)=\frac{(x^1-e_2)}{(e_1-e_2)}\frac{(x^2-f_2)}{(f_1-f_2)},$$
$$e_1<x^1<e_2,\quad f_1<x^2<f_2.$$

Clearly, choosing angle variables on the S_1's, the choice of spherical coordinates corresponds to the graph



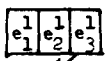
. (3.9)

Only the square of origin of the arrow is of importance for a given arrow connecting two irreducible blocks, not the target square. The general branching law for an arrow connecting two irreducible blocks is readily given:

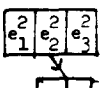


(3.10)

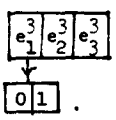
We should also note here that because of the availability of transformations of the type (3.5) some graphs that look different do in fact correspond to the same coordinate system. Indeed, consider graphs of type



(3.11a)



(3.11b)

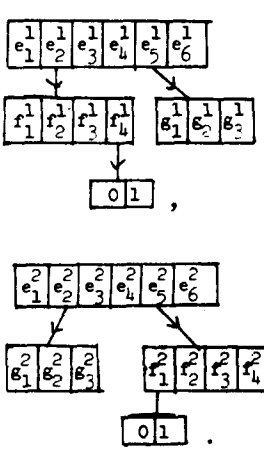


(3.11c)

These graphs correspond to Lamé[9] rotational coordinates on the sphere S_3. There are, however, only two distinct such coordinate systems. In fact, if the coordinates x^i and e_j^1 $(i=1,2, j=1,2,3)$ are subjected to the transformation

$$\begin{aligned} &x^i \to -x^i = y^i; \\ &e_1^1 \to -e_1^1 = e_3^3, \quad e_2^1 \to -e_2^1 = e_2^3, \\ &e_3^1 \to -e_3^1 = e_1^3, \end{aligned} \tag{3.12}$$

we see that the (3.11a) and (3.11c) correspond to the same type of coordinates. Graphs that are related in this way can be recognized by the feature that if the branch below a given irreducible block $\boxed{e_1|\cdots|e_p}$ is obtained from that of another graph by reflection about a vertical at the center of the corresponding $e_1^1 \cdots e_p^1$ block, then the two graphs are equivalent. (We are assuming, of course, that all other features of the graphs are identical.) Graphs that are essentially the same can be related by several transformations of the type (3.5) and the situation gets more complicated, e.g.,



(3.13)

If the two irreducible blocks of S_n and S_p occur as indicated in (3.10), as part of some larger graph, this means that the elliptic coordinates ${}_nu_1,\ldots,{}_nu_{n+1}$ and ${}_pv_1,\ldots,{}_pv_{p+1}$ of these blocks must occur in the combinations

$$\begin{aligned} &w_1 = {}_nu_1,\ldots,w_i = ({}_nu_i)({}_pv_1),\ldots, \\ &w_{i+p+1} = ({}_nu_i)({}_pv_{p+1}), \quad w_{i+p+2} = {}_nu_{i+1},\ldots, \\ &w_{p+n+1} = {}_nu_{n+1}. \end{aligned} \tag{3.14}$$

Arrows may emanate from different squares (e_i's) of the same block but cannot be directed at the same block. With these rules we may construct graphs corresponding to all separable coordinate systems on S_n. For $n=3$, we have the following possibilities[3,4]:

(1) $\boxed{0|1|a|b}$ Jacobi elliptic coordinates, (3.15)

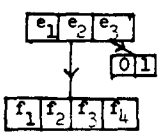
(2) (a) $\boxed{0|1|a}$ $\boxed{0|1}$ (b) $\boxed{0|1|a}$ $\boxed{0|1}$ Lamé rotational coordinates, (3.16)

(3) $\boxed{0|1}$ $\boxed{0|1|a}$ Lamé subgroup reduction, (3.17)

(4) $\boxed{0|1}$ $\boxed{0|1}$ $\boxed{0|1}$ spherical coordinates, (3.18)

(5) $\boxed{0|1}$ $\boxed{0|1}$ $\boxed{0|1}$ cylindrical coordinates. (3.19)

The formation of more complicated graphs is now clear. Thus,



(3.20)

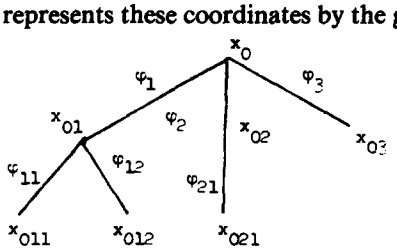
is a coordinate system on S_6 with coordinates

$$\begin{aligned} &s_1^2 = ({}_2u_1)^2, \quad s_2^2 = ({}_2u_2)^2({}_3v_1)^2, \\ &s_3^2 = ({}_2u_2)^2({}_3v_2)^2, \quad s_4^2 = ({}_2u_2)^2({}_3v_3)^2, \\ &s_5^2 = ({}_2u_2)^2({}_3v_4)^2, \quad s_6^2 = ({}_2u_3)^2({}_1w_1)^2, \\ &s_7^2 = ({}_2u_3)^2({}_1w_2)^2. \end{aligned} \tag{3.21}$$

Vilenkin[7] has studied polyspherical coordinates on S_n and developed a graphical technique for constructing them. For example, he considers the coordinates on S_6:

$$\begin{aligned} &x_0 = \cos\varphi_3 \cos\varphi_2 \cos\varphi_1, \\ &x_{03} = \sin\varphi_3, \\ &x_{02} = \cos\varphi_3 \sin\varphi_2 \cos\varphi_{21}, \\ &x_{01} = \cos\varphi_3 \cos\varphi_2 \sin\varphi_1 \cos\varphi_{12} \cos\varphi_{11}, \\ &x_{021} = \cos\varphi_3 \sin\varphi_2 \sin\varphi_{21}, \\ &x_{012} = \cos\varphi_3 \cos\varphi_2 \sin\varphi_1 \sin\varphi_{12}, \\ &x_{011} = \cos\varphi_3 \cos\varphi_2 \sin\varphi_1 \cos\varphi_{12} \sin\varphi_{11}, \end{aligned} \tag{3.22}$$

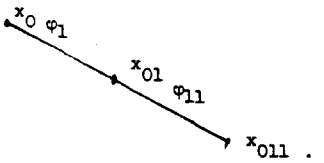
and represents these coordinates by the graph



For him, spherical coordinates on S_2,

$$x_0 = \cos\varphi_1,$$
$$x_{01} = \sin\varphi_1 \cos\varphi_{11}, \tag{3.23}$$
$$x_{011} = \sin\varphi_1 \sin\varphi_{11},$$

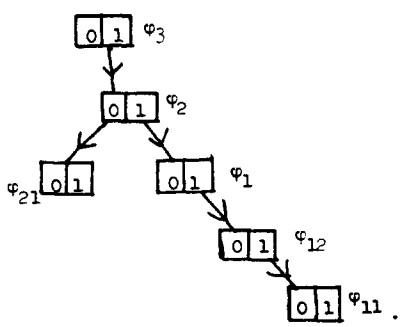
correspond to the graph



Vilenkin denotes coordinates of *rank r* by $x_{0i_1 \cdots i_r}$ and in the example of (3.22) arranges coordinates in the order

$$x_{011}, x_{012}, x_{021}, x_{01}, x_{02}, x_{03}, x_0, \tag{3.24}$$

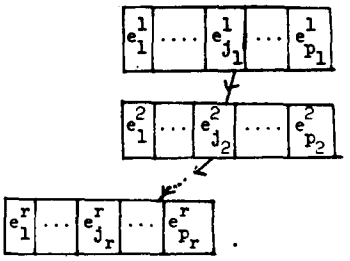
i.e., coordinates of higher rank precede those of lower rank while coordinates of equal rank are ordered lexicographically. Coordinates of the form $x_{0i_1 \cdots i_s j_{s+1} \cdots i_m}$ are called *subordinate* to the coordinate $x_{0i_1 \cdots i_s}$. Further, the coordinate $x_{0j_1 \cdots j_m}$ *essentially precedes* the coordinate $x_{0i_1 \cdots i_s}$ if $m \geqslant s$, and $j_k = i_k$ for $1 \leqslant k \leqslant s-1$ and $j_s < i_s$. The coordinate $x_{0i_1 \cdots i_s}$ *essentially follows* $x_{0j_1 \cdots j_m}$. To extract coordinates on S_n from this notation let $x_{0i_1 \cdots i_m}$ be a vertex of nonzero rank. A rotation $g(\varphi)$ by the angle $\varphi = \varphi_{i_1 \cdots i_m}$ in the $(x_{0i_1 \cdots i_{m-1}}, x_{0i_1 \cdots i_m})$ plane is then associated with this vertex. In this way Vilenkin constructs graphs representing the various possible polyspherical coordinates on S_n. In our notation his coordinate system (3.22) is represented by the graph



From these considerations we see that Vilenkin's polyspherical coordinates are the special case of separable coordinates on S_n consisting of those graphs that contain only the irreducible blocks of type [0|1].

IV. PROPERTIES OF SEPARABLE SYSTEMS IN S_n

Here we make more precise our graphic techniques through a prescription for writing down the standard coordinates s_i, $i = 1,\ldots,n+1$, on S_n in terms of the separable coordinates. A given standard coordinate coming from a given graph consists of a product of r factors, which we denote $x_{p_1 \cdots p_r}^{j_1 \cdots j_r} = ({}_{p_1}u_{j_1}) \cdots ({}_{p_r}u_{j_r})$. This is obtained by tracing the complete length of a branch of a given tree graph, i.e.,



We can then set up an ordering $<$ for the products $x_{P_1 \cdots P_r}^{j_1 \cdots j_r}$. We say that $x_{P_1 \cdots P_r}^{j_1 \cdots j_r} < x_{Q_1 \cdots Q_s}^{i_1 \cdots i_s}$ if $P_1 = Q_1, j_1 = i_1, \ldots, P_t = Q_t, j_t < i_t, P_{t+1} \neq Q_{t+1}, \ldots, j_s \neq i_s$. Then if we arrange the products in increasing order, say $x_1,\ldots,x_{n+1}$, we can identify this ordered n-tuple with $s_1,\ldots,s_{n+1}$. For the example (3.21) given above, the choice of coordinates corresponds to this ordering.

Having settled on a prescription for writing down the coordinates corresponding to a given coordinate system on S_n, we can now discuss the separation equations for both the Hamilton–Jacobi and Helmholtz equations. Let us first consider the coordinates corresponding to the irreducible block [e1|e2|·····|en+1]. The Hamilton–Jacobi equation in these coordinates is

$$H = \sum_{i=1}^{n} \frac{1}{[\Pi_{j \neq i}(x^i - x^j)]} P_i^2 = E, \tag{4.1}$$

where

$$P_i = \left[\prod_{j=1}^{n+1} (x^i - e_j)\right] \frac{\partial S}{\partial x^i}.$$

The separation equations are

$$\left[\prod_{j=1}^{n+1} (x^i - e_j)\right] (\partial_{x^i} S_i)^2 + \left[E(x^i)^{n-1} + \sum_{j=2}^{n} \lambda_j (x^i)^{n-j}\right] = 0. \tag{4.2}$$

If we set $E = \lambda_1$, then the constants of the motion associated with the separation parameters $\lambda_1,\ldots,\lambda_n$ are

$$I_1^n = \sum_{i>j} I_{ij}^2 \quad \text{(second-order Casimir invariant)},$$
$$I_2^n = \sum_{i>j} S_1^{ij} I_{ij}^2, \tag{4.3}$$
$$I_n^n = \sum_{i>j} S_n^{ij} I_{ij}^2,$$

where

$$S_l^{ij} = \frac{1}{l!} \sum_{i_1,\ldots,i_l \neq}{}' e_{i_1} \cdots e_{i_l},$$

and the summation extends over $i_1,\ldots,i_l \neq i, j$ and $i_l \neq i_m$ for $l \neq m$. For the associated Helmholtz equation the eigenvalues of Δ_n have the form $\sigma(\sigma+n-1)$ and the Helmholtz equation becomes

$$\sum_{i=1}^{n} \frac{1}{[\Pi_{j \neq i}(x^i - x^j)]} \left\{\sqrt{\mathscr{P}}_i \frac{\partial}{\partial x^i}\left(\sqrt{\mathscr{P}}_i \frac{\partial \Psi}{\partial x^i}\right)\right\} = -\sigma(\sigma+n-1)\Psi, \tag{4.4}$$

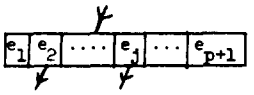
where

$$\mathscr{P}_i = \prod_{j=1}^{n} (x^i - e_j).$$

The separation equations are

$$\sqrt{\mathscr{P}_i}\,\frac{\partial}{\partial x^i}\left(\sqrt{\mathscr{P}_i}\,\frac{\partial \Psi_i}{\partial x^i}\right) + \left[\sigma(\sigma+n-1)(x^i)^n + \sum_{j=2}^{n-1}\tilde{\lambda}_j (x^i)^{n-j}\right]\Psi_i = 0. \tag{4.5}$$

The identification $\tilde{\lambda}_1 = \sigma(\sigma+n-1)$ enables us to further identify the symmetry operators whose eigenvalues are $\tilde{\lambda}_j$ with the expressions (4.3) where $I_{ij}\to\hat{I}_{ij}$ and $[\hat{I}_j^n, \tilde{I}_k^m] = 0$. For an irreducible block appearing in an admissible graph the generalizations of these equations can be computed readily. Consider the block shown as part of a given graph:



Then define $d_i\,(i = 1,\ldots,p+1)$ as follows: $d_i = 0$, if there is no arrow emanating downward from the block $\boxed{e_1}$; otherwise d_i is a parameter.

From the form of the metric we see the variables $x^1,\ldots,x^p$ coming from this block satisfy an equation of the form

$$\sum_{i=1}^{p}\frac{1}{[\Pi_{j\neq i}(x^i - x^j)]}P_i^2 + \sum_{i=1}^{p}\left[\frac{\Pi_{j\neq i}(e_i - e_j)}{\Pi_{j=1}^{p}(x^j - e_i)}\right]d_i = E_p. \tag{4.6}$$

Using the relation

$$\frac{1}{\Pi_{j=1}^{p}(x^j - e_k)} = \frac{1}{\Pi_{i>j}(x^i - x^j)}\left[\sum_{l=1}^{p}\frac{T_l}{(x^l - e_k)}\right], \tag{4.7}$$

where

$$T_l = (-1)^{l+1}\prod_{i>j}{}'(x^i - x^j),$$

with $i,j\neq l$, we see that the separation equations have the form

$$\left[\prod_{j=1}^{p}(x^i - e_j)\right]\left(\frac{dS_i}{dx^i}\right)^2 + \sum_{k=1}^{p+1}\frac{\Pi_{j\neq k}(e_k - e_j)d_k}{(x^i - e_k)} + \left[E_p(x^i)^{p-1} + \sum_{l=2}^{p}\lambda_l (x^i)^{p-l}\right] = 0. \tag{4.8}$$

For the corresponding Helmholtz equation the situation is somewhat more complicated. With each ${}_pu_j$ $(j = 1,\ldots,p+1)$ we associate an index k_j, which is calculated as follows: If the irreducible block occurs as the rth step down from the trunk of the graph and if we write out the S_i in terms of our coordinates then k_j is the number of coordinates for which $x_{p_1\cdots p\cdots p_q}^{j_1\cdots j\cdots j_q}$ (rth column) occurs. The Helmholtz equation assumes the form

$$\sum_{i=1}^{p}\frac{1}{[\Pi_{j\neq i}(x^i - x^j)]}\left\{\sqrt{\frac{\mathscr{P}_i}{\mathscr{Q}_i}}\,\frac{d}{dx^i}\left(\sqrt{\mathscr{P}_i\mathscr{Q}_i}\,\frac{d\Psi}{dx^i}\right)\right\} + \sum_{i=1}^{p}\left[\frac{\Pi_{j\neq i}(e_i - e_j)}{\Pi_{j=1}^{p}(x^j - e_i)}\right]t_i\Psi = -\sigma(\sigma+p-1)\Psi, \tag{4.9}$$

where

$$\mathscr{P}_i = \prod_{j=1}^{p}(x^i - e_j), \quad \mathscr{Q}_i = \prod_{j=1}^{p}(x^i - e_j)^{k_j - 1},$$

$t_i = 0$ if $k_i = 1$ and $t_i = j_i(j_i + k_i - 1)$ if $k_i \neq 1$. The separation equations become

$$\sqrt{\frac{\mathscr{P}_i}{\mathscr{Q}_i}}\,\frac{\partial}{\partial x^i}\left(\sqrt{\mathscr{P}_i\mathscr{Q}_i}\,\frac{\partial \Psi_i}{\partial x^i}\right) + \left\{\sum_{k=1}^{p}\frac{\Pi_{j\neq k}(e_k - e_j)}{(x^i - e_k)}t_k + \left[\sigma(\sigma+p-1)(x^i)^{p-1} + \sum_{l=2}^{p}\tilde{\lambda}_l (x^i)^{p-l}\right]\right\}\Psi_i = 0. \tag{4.10}$$

If we take the coordinates (3.21) and choose

$$\begin{aligned} {}_2u_j^2 &= \frac{\Pi_{i=1}^{2}(x^i - e_j)}{\Pi_{j\neq i}(e_i - e_j)}, \quad j = 1,2,3, \quad i = 1,2, \\ {}_3v_l^2 &= \frac{\Pi_{i=3}^{5}(x^i - f_l)}{\Pi_{m\neq l}(f_m - f_l)}, \quad l = 1,2,3,4, \quad l = 3,4,5, \\ {}_1w_s^2 &= \frac{(x^6 - g_s)}{(g_t - g_s)}, \quad t,s = 1,2, \quad t\neq s, \end{aligned} \tag{4.11}$$

then the separation equations for the Hamilton–Jacobi equation are

$$\begin{aligned} &\text{(i)} \quad \left[\prod_{j=1}^{3}(x^i - e_j)\right]\left(\frac{dS_i}{dx^i}\right)^2 + \frac{(e_2 - e_3)(e_2 - e_1)}{(x^i - e_2)}d_2 + \frac{(e_3 - e_2)(e_3 - e_1)}{(x^i - e_3)}d_3 + Ex^i + \lambda_1 = 0, \quad i = 1,2; \\ &\text{(ii)} \quad \left[\prod_{m=1}^{4}(x^l - f_m)\right]\left(\frac{dS_l}{dx^l}\right)^2 + d_2(x^l)^2 + \lambda_2 x^l + \lambda_3 = 0, \quad l = 3,4,5; \\ &\text{(iii)} \quad \left[\prod_{s=1}^{2}(x^6 - g_s)\right]\left(\frac{dS_6}{ds^6}\right)^2 + d_3 = 0; \end{aligned} \tag{4.12}$$

and for the Helmholtz equation the corresponding separation equations are

$$\text{(i)}\quad \sqrt{\frac{\Pi_{j=1}^{3}(x^i-e_j)}{(x^i-e_2)^3(x^i-e_3)}}\,\frac{d}{dx^i}\left(\sqrt{\prod_{j=1}^{3}(x^i-e_j)(x^i-e_2)^3(x^i-e_3)}\,\frac{d\Psi_i}{dx^i}\right)$$
$$+\left[\frac{(e_3-e_2)(e_3-e_1)}{(x^i-e_3)}j_1(j_1+2)+\frac{(e_3-e_2)(e_3-e_1)}{(x^i-e_3)}j_2^2+j(j+5)x^i+\lambda_1\right]\Psi_i=0,\quad i=1,2;$$

$$\text{(ii)}\quad \sqrt{\prod_{m=1}^{4}(x^l-f_m)}\,\frac{d}{dx^i}\left(\sqrt{\prod_{m=1}^{4}(x^l-f_m)}\,\frac{d\Psi_l}{dx^i}\right)+[l(l+2)(x^l)^2+\lambda_2x^l+\lambda_3]\Psi_l=0,\quad l=3,4,5; \tag{4.13}$$

$$\text{(iii)}\quad \sqrt{\prod_{s=1}^{2}(x^6-g_s)}\,\frac{d}{dx^6}\left(\sqrt{\prod_{s=1}^{2}(x^6-g_s)}\,\frac{d\Psi_6}{dx^6}\right)+j_2^2\,\psi_6=0;$$

$$ds^2=ds_1^2+\cdots+ds_Q^2.$$

Once we are given the coordinates and have computed the associated separation equations for (I) and (II) we can also compute the Killing tensors corresponding to the separation constants: In (4.8) we put $\lambda_1=E_p$. Given ${}_pu_j$, two coordinates s_i,s_k are said to be *connected* if they both contain ${}_pu_j$. The corresponding Killing tensors are then calculated from the formulas (4.3) with I_{ij}^2 replaced by $\Sigma_{r>s}I_{rs}^2$, where the sum extends over all indices r connected to i and s connected to j. The Killing tensors correspond to I_1^m-type operators of the next irreducible block of dimension m connected further up the branch in question. For example, consider the coordinates (3.21). The corresponding Killing tensors are

$$L_1=\sum_{i>j}I_{ij}^2,$$
$$L_2=e_1\left(\sum_{i=2}^{5}I_{6i}^2+I_{7i}^2\right)+e_2\,(I_{16}^2+I_{17}^2)+e_3\left(\sum_{j=2}^{5}I_{ij}^2\right),$$
$$L_3=\sum_{k>l}{}'I_{kl}^2,\quad k,l=2,3,4,5,$$
$$L_4=(f_1+f_2)I_{45}^2+(f_1+f_3)I_{35}^2+(f_1+f_4)I_{34}^2$$
$$+(f_2+f_3)I_{25}^2+(f_2+f_4)I_{24}^2+(f_3+f_4)I_{23}^2, \tag{4.14}$$
$$L_5=f_1f_2I_{45}^2+f_1f_3I_{35}^2+f_1f_4I_{34}^2+f_2f_3I_{25}^2$$
$$+f_2f_4I_{24}^2+f_3f_4I_{23}^2,$$
$$L_6=I_{67}^2.$$

For the Hamilton–Jacobi equation these tensors have the constant values

$$L_1\sim E_1,\quad L_2\sim\lambda_1,\quad L_3\sim d_2,$$
$$L_4\sim\lambda_2,\quad L_5\sim\lambda_3,\quad L_6\sim d_3,$$

and for the Helmholtz equation with $I_{ij}\to\hat{I}_{ij}$ the resulting operators L_i $(i=1,\ldots,6)$ have the eigenvalues $\tilde{L}_1\sim j(j+5)$, $\tilde{L}_2\sim\lambda_1$, $\tilde{L}_3\sim l(l+2)$, $\tilde{L}_4\sim\lambda_2$, $\tilde{L}_5\sim\lambda_3$, $\tilde{L}_6\sim j_2^2$.

V. SEPARATION OF VARIABLES ON R_n

As was the case for S_n all separable coordinate systems in R_n can be chosen to be orthogonal.

Theorem: Let $\{x^i\}$ be a coordinate system on R_n for which the Hamilton–Jacobi equation admits separation of variables and let q be the number of ignorable variables. Then it is always possible to choose an equivalent coordinate system $\{x^i\}$ such that $g^{ij}=\delta^{ij}H_i^{-2}$, i.e., the coordinates are orthogonal. Furthermore, the ignorable variables $\alpha_1,\ldots,\alpha_q$ can always be taken such that

$$p_{\alpha_1}=I_{12},\ldots,p_{\alpha_p}=I_{2p-1,2p}\,p_{\alpha_{p+1}}$$
$$=P_{2p+1},\ldots,p_{\alpha_q}=P_{p+q}.$$

Proof: We use methods similar to those for S_n. Any element of the algebra $\mathscr{E}(n)$ is conjugate to one of the two forms

(1) $L=I_{12}+b_2I_{34}+\cdots b_\nu I_{2\nu-1,2\nu}+\beta P_{2\nu+1}$,

where $\beta=0$ if $n=2\nu$; and

(2) $L'=P_n$.

Let $\{x^i\}$ be a separable system with $q=1$. It follows from the block-diagonal form that this system must be orthogonal. Furthermore, without loss of generality we can assume that $p_{\alpha_1}=L$ or $p_{\alpha_1}=L'$. It is evident that the second case can occur and is in accordance with the statement of the theorem. For the first case we can always choose the ignorable variable α_1 so that it is related to the Cartesian coordinates $(y_1,\ldots,y_n)$ by

$$(y_1,\ldots,y_n)$$
$$=(\rho_1\cos(\alpha_1+w_1),\rho_1\sin(\alpha_1+w_1),\ldots,$$
$$\rho_\nu\cos(b_\nu\alpha_1+w_\nu),$$
$$\rho_\nu\sin(b_\nu\alpha_1+w_\nu),\rho_{\nu+1}+\beta\alpha_1,y_{2\nu+2},\ldots,y_n). \tag{5.1}$$

The infinitesimal metric then has the form

$$ds^2=d\rho_1^2+\cdots+d\rho_\nu^2+\rho_1^2(d\alpha_1+dw_1)^2$$
$$+\cdots+\rho_\nu^2(b_\nu\,d\alpha_1+dw_\nu)^2+(d\rho_{\nu+1}+\beta\,d\alpha_1)^2$$
$$+dy_{2\nu+2}^2+\cdots+dy_n^2. \tag{5.2}$$

If there is only one ignorable variable the coordinate system must be orthogonal and consequently

$$\rho_1^2\,dw_1+\sum_{j=2}^{\nu}b_j\rho_j^2\,dw_j+\beta\,d\rho_{\nu+1}=0. \tag{5.3}$$

This is possible only if $b_2=\cdots=b_\nu=\beta=0$ and $dw_1=0$. (By redefining α_1 we then can take $w_1=0$.) Therefore if we have only one ignorable variable then $p_\alpha=I_{12}$ or P_n.

Now suppose we have q Killing vectors p_{α_i}, $i=1,\ldots,q$. Then they must be of the form

$$
\begin{aligned}
L_1 &= I_{12} + \sum_{l>p}^{s} b_l^1 I_{2l-1,2l} + \sum_{m=2s+1}^{n} \gamma_m^1 P_m,\\
L_2 &= I_{34} + \sum_{l>p}^{s} b_l^2 I_{2l-1,2l} + \sum_{m=2s+1}^{n} \gamma_m^2 P_m,\\
&\vdots\\
L_p &= I_{2p-1,2p} + \sum_{l>p}^{s} b_l^p I_{2l-1,2l} + \sum_{m=2s+1}^{n} \gamma_m^p P_m,\\
L_{p+1} &= \sum_{m=2s+1}^{n} \gamma_m^{p+1} P_m,\\
&\vdots\\
L_q &= \sum_{m=2s+1}^{n} \gamma_m^q P_m.
\end{aligned}
\tag{5.4}
$$

The condition $\{L_i,L_l\}=0$ implies

$$
b_k^i \gamma_{2k-1}^l = b_k^i \gamma_{2k}^l = 0, \tag{5.5}
$$

for $i=1,...,p$, $l=1,...,q$, $k=p+1,...,s$. We are assuming that there is always one b_k^i nonzero for each k and some i. Then $\gamma_{2k-1}^l = \gamma_{2k}^l = 0$ for $k=p+1,...,s$ and $l=1,...,q$. The Cartesian coordinates are

$$
\begin{aligned}
(y_1,...,y_n) = \Big(&\rho_1\cos(\alpha_1+w_1),\rho_1\sin(\alpha_1+w_1),...,\rho_p\cos(\alpha_p+w_p),\rho_p\sin(\alpha_p+w_p),\\
&\rho_{p+1}\cos\Big(\sum_{l=1}^{p} b_{p+1}^l\alpha_l + w_{p+1}\Big),...,\rho_s\sin\Big(\sum_{l=1}^{p} b_s^l\alpha_l + w_s\Big),\sum_{l=1}^{q}\gamma_{2s+1}^l\alpha_l + w_{2s+1},...,\sum_{l=1}^{q}\gamma_n^l\alpha_l + w_n\Big).
\end{aligned}
\tag{5.6}
$$

This set of candidate ignorable variables can take the necessary block-diagonal form only if $dw_i=0$, $b_k^i=0$, for $i=1,...,p$ and $k=p+1,...,s$. Also $dw_l=0$, for $l=2s+1,...,n$. We can thus assume that $w_1=\cdots=w_p=0$, $w_{2s+1}=\cdots=w_n=0$. This implies $\gamma_m^i=0$, for $i=1,...,q$, $m=2s+q-p+1,...,n$, and we can also assume $\gamma_m^i=0$, for $i=1,...,p$ and $m=2s+1,...,2s+q-p+1$. Consequently we can take

$$
\begin{aligned}
&L_1 = I_{12},...,L_p = I_{2p-1,2p},\\
&L_{p+1} = P_{2s+1},...,L_q = P_{2s+q-p},
\end{aligned}
\tag{5.7}
$$

and there are no nonzero elements $g^{\alpha_i\alpha_j}$, $1\leqslant i<j\leqslant q$, in the metric. By a suitable $E(n)$ motion we can always choose $s=p$. All separable coordinates in R_n must be orthogonal. Q.E.D.

To find all possible separable coordinate systems on R_n we proceed in analogy with what we have done for S_n. If we choose orthogonal coordinates in which none of the σ_{ij} are constant functions, then

$$
H_i^2 = X_i\left[\prod_{j\neq i}(x^i-x^j)\right] \quad (i=1,...,n), \tag{5.8}
$$

where, as usual,

$$
ds^2 = \sum_{i=1}^{n} H_i^2 (dx^i)^2.
$$

The conditions $R_{ijji}=0$ are equivalent to (2.16) in which the right-hand side is zero. These conditions have the solution

$$
(1/X_i)^{(n+1)} = 0 \quad (i=1,...,n)
$$

and

$$
\frac{1}{X_i} = \sum_{l=0}^{n} a_l (x^i)^{n-l} = g(x^i).
$$

Again we look for choices of $g(x)$ that are compatible with a positive definite metric. There are only two possibilities:

$$
\begin{aligned}
&\text{(i)}\quad g(x) = \prod_{i=1}^{n}(x-e_i) \quad \text{(elliptic coordinates)},\\
&\qquad e_1 < x^1 < e_2 < \cdots < x^{n-1} < e_n < x^n;
\end{aligned}
\tag{5.9}
$$

$$
\begin{aligned}
&\text{(ii)}\quad g(x) = \prod_{i=1}^{n-1}(x-e_i) \quad \text{(parabolic coordinates)},\\
&\qquad x^1 < e_1 < x^2 < e_2 < \cdots < x^{n-1} < e_{n-1} < x^n.
\end{aligned}
$$

These metrics give coordinates in n dimensions that are the analog of elliptic and parabolic coordinates, familiar in Euclidean spaces of dimension $n=2,3$. To these systems we may associate Cartesian coordinates by

$$
\begin{aligned}
&\text{(i)}\quad y_j^2 = c^2\frac{\Pi_{i=1}^{n}(x^i-e_j)}{\Pi_{i\neq j}(e_i-e_j)}, \quad j=1,...,n, \quad c\in\mathbf{R};\\
&\text{(ii)}\quad y_1 = (c/2)(x^1+\cdots+x^n+e_1+\cdots+e_{n-1}),\\
&\qquad y_j^2 = -c^2\frac{\Pi_{i=1}^{n}(x^i-e_{j-1})}{\Pi_{i\neq j-1}(e_i-e_{j-1})}, \quad j=2,...,n.
\end{aligned}
\tag{5.10}
$$

These two systems are fundamental for generating all separable systems on R_n. As an example of the relevance of these systems we consider the case when some of the σ_{ij} functions are constants. We first treat, as we did for S_n, the

case in which the metric coefficients have the form (2.22) and (2.23). Then, as we have shown, these coefficients reduce to

$$H_i^2 = \left[X_i \prod_{j\neq i}(x^i - x^j)\right]\left(\prod_{h=k+1}^{n}\sigma_h\right),$$
$$H_l^2 = \left[X_l \prod_{m\neq l}(x^l - x^m)\right]. \tag{5.11}$$

The conditions $R_{klik} = 0$ imply that the quadratic form

$$ds'^2 = \sum_l H_l^2 (dx^l)^2$$

is that of a flat space. The remaining nonzero conditions are

$$\tilde{H}_i^{-2}\tilde{H}_j^{-2}\tilde{R}_{ijji} + \left(\prod_{l=k+1}^{n}\sigma_l\right)\left[\sum_{m=k+1}^{n}\frac{1}{4H_m^2}\left(\frac{\sigma_m'}{\sigma_m}\right)^2\right] = 0, \tag{5.12}$$

$$2\frac{\sigma_l''}{\sigma_l} - \left(\frac{\sigma_l'}{\sigma_l}\right)^2 - \left(\frac{\sigma_l'}{\sigma_l}\right) \times\left[\frac{\partial}{\partial x^l}\log H_l^2 + H_l^2\sum_{m\neq l}\frac{1}{H_m^2(x^l - x^m)}\right] = 0, \tag{5.13}$$

with $\tilde{R}_{ijji}$ as in (2.25). These equations are satisfied provided $\tilde{R}_{ijji} = -\tilde{H}_i^2\tilde{H}_j^2$ and the function $\Sigma = (\Pi_{l=k+1}^{n}\sigma_l)$ is given as follows:

$$\frac{1}{X_l} = \prod_{m=k+1}^{N}(x^m - e_l), \quad l = k+1,\ldots,n, \tag{5.14}$$

$$\Sigma = \frac{\Pi_{l=k+1}^{N}(x^l - e_m)}{\Sigma_{l\neq m}(e_l - e_m)}, \quad \text{for some } m \text{ fixed}, \tag{5.15}$$

where $N = n, n-1$. The functions $1/X_i$ are given by

$$\frac{1}{X_i} = -4\prod_{j=1}^{k+1}(x^i - e_j'). \tag{5.16}$$

The systems are related to Cartesian coordinates on R_n according to

$$(y_1,\ldots,y_n) = (w_1 s_1,\ldots,w_1 s_{k+1}, w_2,\ldots,w_{n-k}), \tag{5.17}$$

where

$$\sum_{i=1}^{k+1} s_i^2 = 1 \quad \text{and} \quad s_j^2 = \frac{\Pi_{i=1}^{k}(x^i - e_j')}{\Pi_{j\neq i}(e_i' - e_j')},$$

$$\text{(i)} \quad w_l^2 = \frac{\Pi_{m=1}^{n-k}(x^m - e_l)}{\Pi_{m\neq l}(e_m - e_l)}, \quad l = 1,\ldots,n-k;$$

$$\text{(ii)} \quad w_l^2 = \frac{\Pi_{m=1}^{n-k}(x^m - e_l)}{\Pi_{m\neq l}(e_m - e_l)}, \quad l = 1,\ldots,n-k-1, \tag{5.18}$$

$$w_{n-k} = \frac{1}{2}\left(\sum_{m=1}^{n-k}x^m + e_1 + \cdots + e_{n-k}\right).$$

There exists an additional possibility that could be discounted for S_n: $\sigma_l = a_l$, $l = k+1,\ldots,n$. This corresponds to the case in which the infinitesimal distance can be written

$$ds^2 = ds_1^2 + ds_2^2, \tag{5.19}$$

where ds_1^2 is the infinitesimal distance for elliptic or parabolic coordinates in R_k and ds_2^2 is a similar infinitesimal distance on R_{n-k}. We can mimic the procedure adopted for S_n. The only essential difference is that the infinitesimal distance can be expressed, in general, as a sum of distances that can be identified with Euclidean subspaces. This reflects the fact that if $\{y^i\}$, $i = 1,\ldots,n_1$, and $\{z^j\}$, $j = 1,\ldots,n_2$, are separable coordinate systems in Euclidean spaces R_{n_1} and R_{n_2} with respective infinitesimal distances ds_1^2, ds_2^2, then the coordinates $\{y^i, z^j\}$, $i = 1,\ldots,n_1$, $j = 1,\ldots,n_2$, can be regarded as a separable coordinate system on $R_{n_1+n_2}$ with corresponding infinitesimal distance $ds^2 = ds_1^2 + ds_2^2$. This is, of course, not the case for S_n. This property of Euclidean space coordinates naturally extends to separable coordinate systems $\{x_p^i\}$, $i = 1,\ldots,n_p$, $p = 1,\ldots,Q$, on R_p in such a way that

$$ds^2 = ds_1^2 + \cdots + ds_Q^2.$$

In general the infinitesimal distance can be written as a sum of basic forms

$$ds^2 = \sum_{I=1}^{Q} ds_I^2, \tag{5.20}$$

where

$$ds_I^2 = \sum_{i=1}^{n_I}\left[\frac{\Pi_{l=1}^{N_I}(x^l - e_i^I)}{\Pi_{j\neq i}(e_j^I - e_i^I)}\right]d\omega_i^2 + d\sigma_I^2. \tag{5.21}$$

Here the $d\sigma_I^2$ is the infinitesimal distance corresponding to elliptic or parabolic coordinates for a flat space of dimension N_I. Also $n_I \leqslant N_I$ for elliptic coordinates with a strict inequality for parabolic coordinates.

The $d\omega_i^2$ is the infinitesimal distance of some separable coordinate system on the sphere S_{p_I} and $n = \Sigma_{I=1}^{Q}(N_I + p_I)$. To establish a graphic procedure for construction of separable coordinates we need only analyze one of the basic forms ds_I^2. We should also mention here that if $N_I = 1$, then the basic form is written

$$ds_I^2 = w^2\,d\omega^2 + dw^2. \tag{5.21'}$$

A basic form could in fact correspond to elliptic or parabolic coordinates on R_{N_I} and no $d\omega_i^2$ terms. We associate this with $n_I = 0$ in (5.21).

For our construction we need only invent graphic representations for elliptic and parabolic coordinates in R_n, the analog of the irreducible blocks on S_n. We adopt the following notation:

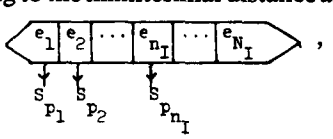
(1) elliptic coordinates 

, $n \geqslant 1$,

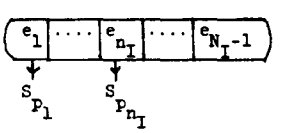
(2) parabolic coordinates 

, $n \geqslant 2$.

It is clear that only elliptic coordinates exist in one dimension. The graphical representation of a basic form corresponding to the infinitesimal distance ds_I^2 has the appearance

(i) 

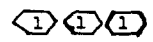
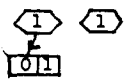
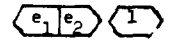
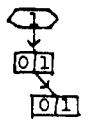
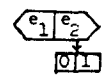
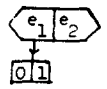
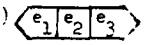
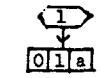
,

(ii) 

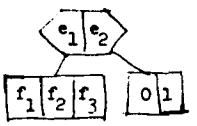
.

Attached to each leg descending from the top block is the appropriate graph of the coordinate system on the S_{p_i} giving

TABLE I. Separable systems for R_3.

1) 	Cartesian coordinates
2) 	cylindrical coordinates
3) 	elliptic cylindrical
4) 	parabolic cylindrical
5) 	spherical coordinates
6) 	prolate spheroidal
7) 	oblate spheroidal
8) 	parabolic coordinates
9) 	paraboloidal coordinates
10) 	ellipsoidal coordinates
11) 	conical coordinates

rise to the form $d\omega_i^2$. The general graph corresponding to a separable system then can be constructed as a sum of disconnected graphs for basic forms. We first illustrate this technique for the separable systems of R_3 (see Ref. 21) (see Table I). As an additional nonstandard example, consider the graph



which defines a coordinate system in R_5. The coordinates can be chosen as

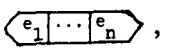
$$y_i^2 = c^2\left[\frac{(x^1-e_1)(x^2-e_1)}{(e_2-e_1)}\right](_2u_i)^2, \quad i=1,2,3,$$
$$y_4^2 = c^2\left[\frac{(x^1-e_2)(x^2-e_2)}{(e_1-e_2)}\right]\cos^2 x^5, \tag{5.22}$$
$$y_5^2 = c^2\left[\frac{(x^1-e_2)(x^2-e_2)}{(e_1-e_2)}\right]\sin^2 x^5,$$

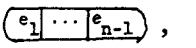
where

$$(_2u_i)^2 = \frac{(x^3-f_k)(x^4-f_l)}{(f_j-f_l)(f_k-f_l)}, \quad i,j,k \text{ distinct.}$$

We can set up a natural ordering for separable systems in R_n. For a given basic form we can suppose the natural ordering of the e_i's in the leading irreducible block on the ordering of the S_{p_i} branches and then write down coordinates in a standard way.

The ordering of the disconnected parts of the graph is presumed already given. There are equivalences (relating graphs of various coordinate systems) that we have already discussed for the n-sphere and, of course, there is an additional equivalence corresponding to the permutation of disconnected parts of a given graph. The separation equations can be readily computed also. For the elliptic and parabolic coordinate blocks

(1)  ,

(2)  ,

the Hamilton–Jacobi equation has the form

$$H = \sum_{i=1}^{n} \frac{1}{[\Pi_{j\neq i}(x^i-x^j)]} P_i^2 = E, \tag{5.23}$$

where

$$P_i = \left[\prod_{j=1}^{N_k}(x^i-e_j)\right]\frac{\partial S}{\partial x^i},$$

with $N_1 = n$ (elliptic coordinates) and $N_2 = n-1$ (parabolic coordinates). The separation equations are

$$\left[\prod_{j=1}^{N_k}(x^i-e_j)\right](\partial_{x^i}S_i)^2$$
$$+\left[E(x^i)^{n-1}+\sum_{j=2}^{n}\lambda_j(x^i)^{n-j}\right]=0. \tag{5.24}$$

If we identify $E=\lambda_1$, the constants of the motion associated with the separation parameters $\lambda_1,\ldots,\lambda_n$ are

$$_1I_1^n = P_1^2+\cdots+P_n^2,$$
$$_1I_2^n = \sum_{i>j} I_{ij}^2 + c^2\sum_{i=1}^{n} S_1^i P_i^2, \tag{5.25a}$$
$$\vdots$$
$$_1I_n^n = \sum_{i>j} S_{n-2}^{ij} I_{ij}^2 + c^2\sum_{i=1}^{n} S_{n-1}^i P_i^2,$$

where

$$S_l^i = \frac{1}{l!}\sum_{i_1,\ldots,i_l\neq} e_{i_1}\cdots e_{i_l}$$

and the sum is over $i_1,\ldots,i_l\neq i$; and

$$
\begin{aligned}
{}_2I_1^n &= P_1^2 + \cdots + P_n^2,\\
{}_2I_2^n &= c\sum_{k=2}^{n}\{I_{1k},P_k\} + c^2S_1P_1^2 + \sum_{j=2}^{n} c^2S_1^jP_j^2,\\
{}_2I_3^n &= \sum_{k=2}^{n} cS_1^k\{I_{1k},P_k\} + \sum_{i>j>2} I_{ij}^2\\
&\quad + c^2S_2P_1^2 + c^2\sum_{j=2}^{n} S_2^jP_j^2, \qquad (5.25b)\\
{}_2I_4^n &= \sum_{k=2}^{n} cS_2^k\{I_{1k},P_k\} + \sum_{i>j>2} S_1^{ij}I_{ij}^2\\
&\quad + c^2S_3P_1^2 + c^2\sum_{j=2}^{n} S_3^jP_j^2,\\
&\vdots\\
{}_2I_n^n &= \sum_{k=2}^{n} cS_{n-2}^k\{I_{1k},P_k\} + \sum_{i>j>2} S_{n-3}^{ij}I_{ij}^2\\
&\quad + c^2S_{n-1}P_1^2,
\end{aligned}
$$

where the S_n^j have the same significance as for elliptic coordinates and

$$S_l = \frac{1}{l!}\sum_{i_1,\ldots,i_l\neq} e_{i_1}\cdots e_{i_l}.$$

For the corresponding Helmholtz equation the eigenvalues of Δ_n are $-k^2$ (k real) and the Helmholtz equation reads

$$\sum_{i=1}^{n}\frac{1}{[\Pi_{j\neq i}(x^i-x^j)]}\left\{\sqrt{\mathscr{P}_i}\,\frac{\partial}{\partial x^i}\left(\sqrt{\mathscr{P}_i}\,\frac{\partial\Psi}{\partial x^i}\right)\right\} = -k^2\Psi, \qquad (5.26)$$

where $\mathscr{P}_i = \Pi_{j=1}^{N_k}(x^i-e_j)$. The separation equations are

$$\sqrt{\mathscr{P}_i}\,\frac{\partial}{\partial x^i}\left(\sqrt{\mathscr{P}_i}\,\frac{\partial\Psi_i}{\partial x^i}\right) + \left[k^2(x^i)^n + \sum_{j=2}^{n-1}\lambda_j(x^i)^{n-j}\right]\Psi_i = 0. \qquad (5.27)$$

For a basic form such as ds_I^2 the separation equations for the Hamilton–Jacobi equation have the form

$$\left[\prod_{j=1}^{N_{I_k}}(x^i-e_j)\right]\left(\frac{\partial S_i}{\partial x^i}\right)^2 + \sum_{l=1}^{n_I}\frac{\Pi_{j\neq k}(e_l-e_j)}{(x^i-e_l)}k_l + \left[E_I(x^i)^{N_{I_k}-1} + \sum_{l=2}^{N_{I_k}}\lambda_l(x^i)^{N_{I_k}-l}\right] = 0, \qquad (5.28)$$

where k_l is the constant value of the Hamiltonian on the sphere whose infinitesimal distance is $d\omega_l^2$. For the Helmholtz equation the corresponding contribution of this basic form is the equation

$$\sum_{i=1}^{N_{I_k}}\frac{1}{[\Pi_{j\neq i}(x^i-x^j)]}\left[\sqrt{\frac{\mathscr{P}_i}{\mathscr{Q}_i}}\,\frac{\partial}{\partial x^i}\left(\sqrt{\mathscr{P}_i\mathscr{Q}_i}\,\frac{\partial\Psi}{\partial x^i}\right) + \sum_{i=1}^{n_I}\left[\frac{\Pi_{j\neq i}(e_i-e_j)}{\Pi_{j=1}^{n_{I_k}}(x^j-e_i)}\right]j_i(j_i+p_i-1)\Psi\right] = -k_I^2\Psi, \qquad (5.29)$$

where

$$\mathscr{P}_i = \prod_{k=1}^{N_{I_k}}(x^i-e_k), \quad \mathscr{Q}_i = \prod_{k=1}^{N_{I_k}}(x^i-e_k)^{d_k-1},$$

$$d_k = \begin{cases} p_k+1, & \text{if } k=1,\ldots,n_I,\\ 1, & \text{if } k=n_I+1,\ldots,N_{I_k}.\end{cases}$$

The separation equations are

$$\sqrt{\frac{\mathscr{P}_i}{\mathscr{Q}_i}}\,\frac{d}{dx^i}\left(\sqrt{\mathscr{P}_i\mathscr{Q}_i}\,\frac{d\Psi_i}{dx^i}\right) + \left[\sum_{k=1}^{n_I}\left[\frac{\Pi_{j\neq k}(e_k-e_j)}{(x^i-e_k)}\right]j_i(j_i+p_i-1) + k_I^2(x^i)^{N_{I_k}-1} + \sum_{l=2}^{N_{I_k}}\lambda_l(x^i)^{N_{I_k}-l}\right]\Psi_i = 0. \qquad (5.30)$$

In the example on R_5 the separation equations for the Hamilton–Jacobi equation are

$$\left[\prod_{j=1}^{2}(x^i-e_j)\right]\left(\frac{dS_i}{dx^i}\right)^2 + \frac{(e_2-e_1)}{(x^i-e_2)}k_1 + \frac{(e_1-e_2)}{(x^i-e_1)}k_2 + k^2x^i + \lambda_1 = 0, \quad i=1,2, \qquad (5.31)$$

and for the Helmholtz equation they are

$$\sqrt{\frac{\Pi_{j=1}^{2}(x^i-e_j)}{(x^i-e_1)^2(x^i-e_2)}}\,\frac{d}{dx^i}\times\left[\prod_{j=1}^{2}(x^i-e_j)(x^i-e_1)^2(x^i-e_2)\,\frac{d\Psi_i}{dx^i}\right] + \left[\frac{(e_2-e_1)}{(x^i-e_2)}j_1^2 + \frac{(e_1-e_2)}{(x^i-e_1)}j_2(j_2+1) + k^2x^i + \tilde{\lambda}_1\right]\Psi_i = 0. \qquad (5.32)$$

For the elliptic case the only new prescription required is that P_i^2 be replaced by $\Sigma_r P_r^2$, where the sum extends over all induces r connected to i. Similar comments apply to expressions of the form $\{I_{kl},P_l\}$.

For our example the operators that describe separation are

$$
\begin{aligned}
L_1 &= I_{12}^2 + I_{23}^2 + I_{13}^2,\\
L_2 &= f_1I_{23}^2 + f_2I_{13}^2 + f_3I_{12}^2,\\
L_3 &= I_{45}^2, \qquad (5.33)\\
L_4 &= \sum_{i=1}^{5} P_i^2,\\
L_6 &= \sum_{i=1}^{3}(I_{i4}^2 + I_{i5}^2)\\
&\quad + c^2[e_2(P_1^2+P_2^2+P_3^2) + e_1(P_4^2+P_5^2)].
\end{aligned}
$$

The operator L_6 corresponds to the separation constant λ_1.

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An inverse problem for multidimensional first-order systems

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An inverse problem associated with N first-order equations in $n+1$ dimensions, $n>1$, is considered: Given appropriate inverse data T reconstruct the potential $q(x_0,x)$, where q is an $N\times N$ off-diagonal matrix. Although q depends on $n+1$ variables, it turns out that T depends on $3n-1$ variables. This necessitates imposing certain constraints on T, i.e., T must be suitably characterized. The characterization problem for T is solved explicitly. Furthermore, the problem of reconstructing q is reduced to one for reconstructing a 2×2 matrix potential in two dimensions. The inverse data needed for the reduced problem are obtained in closed form from T. A method for solving two-dimensional inverse problems has recently appeared in the literature.

I. INTRODUCTION

In this paper we shall study the inverse problem associated with the following system of N first-order equations in $n+1$ dimensions:

$$\Psi_{x_0}+\sigma\sum_{l=1}^{n}J_l\Psi_{x_l}=q\Psi,$$
$$\sigma=\sigma_R+i\sigma_I,\quad \sigma_I\neq 0,\quad n>1, \tag{1.1}$$

where $q(x_0,x)$ is an $N\times N$ matrix-valued off-diagonal function in $\mathbb{R}^{n+1}$, decaying suitably fast for large x_0, x, and the J_l are constant real diagonal $N\times N$ matrices (we denote the diagonal entries of J_l by $J_l^1,\ldots,J_l^N$). Alternatively, using the transformation

$$\Psi(x_0,x,k)=\mu(x_0,x,k)\exp\left[i\sum_{l=1}^{n}k_l(x_l-\sigma x_0 J_l)\right],\quad k\in\mathbb{C}^n, \tag{1.2}$$

we shall study

$$\mu_{x_0}+\sigma\sum_{l=1}^{n}(J_l\mu_{x_l}+ik_l[J_l,\mu])=q\mu. \tag{1.3}$$

We assume that $n\leqslant N$, otherwise the entries of the J_l matrices will be linearly related and one can always reduce n by a change of coordinates. An inverse problem in this case is defined as follows: Given appropriate *inverse data* T, where T is an $N\times N$ matrix-valued off-diagonal function of suitable *inverse parameters*, reconstruct the potential q.

There is a twofold motivation for considering such an inverse problem.

(a) If $\sigma=-1$ then the above reduces to the formulation of a physically important inverse scattering problem: Given the *scattering amplitude* $S(\lambda,k)$, λ, $k\in\mathbb{R}^n$, which is a function of the *scattering parameters* λ, k, reconstruct q.

(b) In recent years a deep connection has been discovered[1] between inverse scattering of linear eigenvalue problems in one spatial dimension and the initial value problem of certain nonlinear evolution equations in $1+1$ (i.e., one spatial and one temporal dimension). This is the essence of the celebrated inverse scattering transform (IST) method. The inverse scattering of the time-independent Schrödinger and of the Dirac eigenvalue equations[2] have been used to linearize the Korteweg–de Vries (KdV),[1] nonlinear Schrödinger,[3] modified KdV,[2] and sine–Gordon[2] equations. Several other equations also have been linearized using similar principles.[4,5] Recently a similar connection has been used to extend the above results to nonlinear evolution equations in $2+1$ (i.e., two spatial and one temporal dimension).[6–10] In particular the *inverse scattering* of (1.3) with $\sigma=-1$ and $n=1$ has been used to linearize the N-wave interaction equations in $2+1$ (see Ref. 8), the Davey–Stewartson (DS) I (see Ref. 8) (a $2+1$ analog of the nonlinear Schrödinger), and the modified Kadomtsev–Petviashvili (MKP) I (see Ref. 8) (a $2+1$ analog of the modified KdV) equations. Furthermore the *inverse problem* of (1.3) with $\sigma=i$ and $n=1$ has been used to linearized[9] DSII and MKP II. However, in spite of the above success in $2+1$, no physically interesting equation is known to be related to (1.3) for $n>1$ and $\sigma_I\neq 0$ [the N-wave interaction equations in $n+1$ spatial and one temporal dimension[11] are related to (1.3) but with $\sigma_I=0$].

The novelty associated with inverse problems in greater than two spatial dimensions ($n>1$) stems from the fact that while the potential $q(x_0,x)$ depends on $n+1$ variables, the inverse data $T(k_R,k_I,m_2,\ldots,m_n)$, $k_R\in\mathbb{R}^n$, $k_I\in\mathbb{R}^n$, $m_l\in\mathbb{R}$, depends on $3n-1$ variables. This has important implications.

(a) The inverse data must be appropriately constrained. This "characterization" of the inverse data is conceptually analogous to the characterization of the inverse scattering data in the multidimensional Schrödinger equation.[12–15]

(b) The existence of "redundant" scattering parameters in the inverse scattering of the Schrödinger equation is used to reconstruct the potential in *closed form* in terms of the scattering amplitude function. This is the well-known Born approximation.[16] Can one use the redundancy of the inverse parameters here to also reconstruct q in closed form?

In this paper, we do the following.

(a) We derive an equation that characterizes inverse data [see (4.13)]:

$$\hat{T}^{ij}(w_0,w)\doteq T^{ij}(w_0,w,\chi)-\frac{1}{\pi}\int_{\mathbb{R}^2}\frac{d\chi'_{P_R}\,d\chi'_{P_I}N^{ij}_{lP}[T](w_0,w,\chi^{P'})}{\chi_P-\chi'_P}, \tag{1.4}$$

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where $w_0 \in \mathbb{R}$, $w \in \mathbb{R}^n$, $\chi \in \mathbb{C}^{n-1}$ are related to k, m [see (4.5)] and N is a quadratic function of T [see (4.1)]. That is, $T^{ij}(k,m)$ is appropriate inverse data iff the right-hand side of (1.4) is independent of χ. Hence, Eq. (1.4) serves as both characterizing T^{ij} and defining $\hat{T}^{ij}$.

(b) We reduce the general problem of reconstructing an $N \times N$ potential q in $n+1$ dimensions to one of reconstructing a 2×2 potential with entries q^{ij}, q^{ji} in two dimensions. The inverse data needed for this reconstruction is precisely $\hat{T}^{ij}$, $\hat{T}^{ji}$. This reduction makes crucial use of the existence of redundant scattering parameters. In this sense it is the analog of the Born approximation.

In more detail this paper is organized as follows: In Sec. II we introduce an eigenfunction $\mu(x_0,x,k)$ bounded for all $k \in \mathbb{C}^n$. We assume that μ has no homogeneous solutions, otherwise the formalism presented here must be suitably modified in a manner similar to that used in two spatial dimensions.[9] The departure of μ from holomorphicity is measured by $\partial\mu/\partial\bar{k}$, which, using a crucial symmetry condition of the underlying Green's function, can be expressed in terms of μ and appropriate inverse data T (see Proposition 2.3). Using a $\bar{\partial}$ formulation one may obtain μ and q in terms of T (Proposition 2.4). The above formulas, which are natural generalizations of the analogous formulas in two spatial dimensions,[8] provide a *less* effective way of reconstructing q than the one given in Sec. V but they provide the basis for the solution of the characterization problem. In Sec. III we formulate a solution to the characterization problem that is analogous to the "miracle condition" of Newton for the characterization of the inverse scattering data in the Schrödinger equation[13]: One has n different ways of reconstructing q in terms of T; furthermore it appears that the reconstructed q depends on k. It is explicitly shown here that the equality of the inversion formulas is equivalent to q being independent of k (Proposition 3.1). Also this equality imposes constraints on T, which, however, depend on μ (which in turn depends on T). Hence, this characterization is *implicit*. In Sec. IV we derive an *explicit* characterization on T (Proposition 4.2). This crucial result uses Proposition 2.3 and the existence of redundant inverse parameters. In Sec. V we use the results of Sec. IV and a suitable coordinate transformation to reduce the problem of reconstructing q to one of reconstructing a 2×2 matrix potential in two spatial dimensions. This reduced problem was solved in Ref. 8.

Equation (1.3) with $\sigma = i$ was first considered in Ref. 17, but neither the characterization problem was solved, nor the reduction to a 2×2 problem in two dimensions was obtained (in other words, some of the results of Sec. II for $\sigma = i$ are given in Ref. 17). Equation (1.3) was also considered in Ref. 18. In particular, the authors of Ref. 18 introduced for the first time the "T-equation," which is essentially Eq. (4.1) of this paper. The introduction of this equation is, in our opinion, a new, fundamental idea in the field of inverse scattering and inverse problems: It provides a powerful approach to an explicit characterization of the inverse data. However, the above authors overlooked the fact that the coefficient ϵ^{lji} of χ appearing in the exponential defining T^{ij} is zero for both $l = i$ and $l = j$. This fact implies that $\hat{T}^{ij}$ [see (1.4)] does not equal the Fourier transform of q^{ij} and hence one cannot obtain a closed form solution for q^{ij} in terms of T^{ij}. For completeness of comparison we also point out that here we use a slightly different formulation of the "symmetry condition" of the underlying Green's functions. This leads to a somewhat simpler formulation of the T-equation.

The physically interesting hyperbolic case $\sigma = -1$ can be considered as a limiting case $\sigma \to -1 + i0^+$. Although this limit exists (see Ref. 18), it turns out to be advantageous to consider the hyperbolic case directly. In Ref. 19 the following results are obtained: (a) the characterization problem of the inverse data is explicitly solved using the analyticity of the underlying eigenfunctions; (b) the problem of reconstructing q is again reduced to reconstructing a 2×2 potential matrix in two dimensions; and (c) a very simple relationship is found between the inverse data T and the scattering amplitude function S. Actually if $N = 3$ then $T = S$.

The results presented here are formal. Both the direct and inverse problems involve linear integral equations. One still needs to establish existence and uniqueness of the solution of these equations. Thus, strictly speaking, "solved" should be replaced by "formally solved." However, if $q(x_0,x)$ decays sufficiently fast for large x_0,x and if its appropriate norm is sufficiently small, all equations presented here are well defined and we expect that these formal results can be made rigorous.

II. THE INVERSE PROBLEM

Proposition 2.1: The solution of (1.3), bounded for all complex values of k and tending to I for large k, is given by

$$\mu^{ij}(x_0,x,k) = \delta^{ij} + \operatorname{sgn}\frac{(\sigma_I J_1^i)}{2\pi i}\int_{\mathbb{R}^2} d\xi_0\, d\xi_1 \frac{\exp[i\beta^{ij}(x_0-\xi_0,\ x_1-\xi_1,\ k)]}{(x_1-\xi_1)-\sigma J_1^i(x_0-\xi_0)} \times (q\mu)^{ij}(\xi_0,\xi_1,x_2-(x_1-\xi_1)J_2^i/J_1^i,\ldots,x_n-(x_1-\xi_1)J_n^i/J_1^i,k), \quad k\in\mathbb{C}^n, \tag{2.1}$$

where β^{ij} is defined by

$$\beta^{ij}(x_0,x_1,k) \doteq \sum_{l=1}^{n} \frac{J_l^i - J_l^j}{\sigma_I}\left[x_0|\sigma|^2 k_{l_I} - \frac{x_1(\sigma k_l)_I}{J_1^i}\right], \quad k_l = k_{l_R} + ik_{l_I}. \tag{2.2}$$

Equivalently μ^{ij} satisfies

$$\mu^{ij}(x_0,x,k)=\delta^{ij}+\frac{\operatorname{sgn}(\sigma_I J_1^i)}{2\pi i}\int_{\mathbf{R}^{n+1}} d\xi_0\, d\xi\left[c_{n-1}\int_{\mathbf{R}^{n-1}} dm^2\, e^{i\alpha^i(x-\xi,m)}\right]\frac{\exp[i\beta^{ij}(x_0-\xi_0,x_1-\xi_1,k)](q\mu)^{ij}(\xi_0,\xi,k)}{x_1-\xi_1-\sigma J_1^i(x_0-\xi_0)}, \tag{2.3}$$

where

$$dm^2\doteq dm_2\cdots dm_n,\quad \alpha^i(x,m)\doteq\sum_{l=2}^{n} m_l\left(x_l-x_1\frac{J_l^i}{J_1^i}\right),\quad c_n\doteq\frac{1}{(2\pi)^n}. \tag{2.4}$$

To derive the above note that the Fourier transform

$$\tilde{\Psi}(x_0,m,k)=\int_{\mathbf{R}^n} d\xi\,\Psi(x_0,\xi,k)\exp(-im\,\xi),$$

of Eq. (1.1) implies that Ψ satisfies

$$\Psi(x_0,x,k)=c_n\int_{\mathbf{R}^n} dm\,\exp[i(mx-\sigma x_0 mJ)]A(m,k)$$
$$+c_n\int_{-\infty}^{x_0} d\xi_0\int_{\mathbf{R}^{2n}} d\xi\,dm\,\exp[im(x-\xi)-i\sigma(x_0-\xi_0)mJ](q\Psi)(x_0,\xi,k), \tag{2.5}$$

where $A(m,k)$ is an arbitrary function of m,k. Hence μ satisfies

$$\mu(x_0,x,k)=c_n\int_{\mathbf{R}^n} dm\,\exp[i(mx-\sigma x_0 mJ-\sigma x_0 k\hat{J})]A(m,k)$$
$$+c_n\int_{-\infty}^{x_0} d\xi_0\int_{\mathbf{R}^{2n}} d\xi\,dm\,\exp[im(x-\xi)-i\sigma(x_0-\xi_0)mJ-i\sigma(x_0-\xi_0)k\hat{J}](q\mu)(x_0,\xi,k), \tag{2.6}$$

where

$$mx\doteq\sum_{l=1}^{n} m_l x_l,\quad mJ\doteq\sum_{l=1}^{n} m_l J_l,\quad \hat{J}_l f=[J_l,f],\quad e^{\hat{J}_l}f=e^{J_l}fe^{-J_l}. \tag{2.7}$$

The exponential of the second term of the right-hand side of (2.6) involves

$$P^{ij}\doteq i\sum_{l=1}^{n}\{m_l(x_l-\xi_l)$$
$$-\sigma[J_l^i m_l+(J_l^i-J_1^i)k_l](x_0-\xi_0)\}.$$

The real part of P^{ij} is given by

$$P_R^{ij}=\sum_{l=1}^{n}[\sigma_I J_l^i m_l+(J_l^i-J_1^i)(\sigma k_l)_I](x_0-\xi_0)$$
$$\doteq[\sigma_I J_1^i m_1+\tilde{P}_R^{ij}](x_0-\xi_0).$$

The second term of the right-hand side of Eq. (2.6) also involves the integral $\int_{-\infty}^{x_0} d\xi_0\int_{-\infty}^{\infty} dm_1$, which equals

$$\int_{-\infty}^{x_0} d\xi_0\int_{-\infty}^{M_1} dm_1-\int_{x_0}^{\infty} d\xi_0\int_{M_1}^{\infty} dm_1+\int_{\mathbf{R}^1} d\xi_0\int_{M_1}^{\infty} dm_1,$$

for arbitrary M_1. Since the third term above can be canceled out of (2.6) with an appropriate choice of $A(m,k)$, it follows that one can always achieve boundedness of μ for all complex values of k: Choose M_1 such that P_R^{ij} is less than zero in $\int_{-\infty}^{x_0} d\xi_0$ and greater than zero in $\int_{x_0}^{\infty} d\xi_0$, i.e., $M_1=-\tilde{P}_R^{ij}/(\sigma_I J_1^i)$ for $\sigma_I J_1^i>0$ (otherwise change sign). The m_1 integration can be performed explicitly: The coefficient of m_1 in P^{ij} is $i[(x_1-\xi_1)-\sigma J_1^i(x_0-\xi_0)]$, hence this quantity will appear in the denominator. Also P^{ij} evaluated at $m_1=M_1$ becomes

$$i\left\{\sum_{l=2}^{n} m_l(x_l-\xi_l)-(x_1-\xi_1)\frac{J_l^i}{J_1^i}\right.$$
$$\left.+\beta^{ij}(x_0-\xi_0,x_1-\xi_1,k)\right\}.$$

Hence (2.6) yields Eq. (2.3). Equation (2.1) follows from Eq. (2.3) by using the fact that the integral over dm^2 is a product of δ functions with arguments $\xi_l=x_l-(x_1-\xi_1)J_l^i/J_1^i$.

Remarks: (1) Equation (2.1) with $n=1$ is equivalent to the analogous one of two-spatial dimensions, e.g., Eq. (4.4) of Ref. 9. Equation (2.1) actually appears simpler because the m_1 integration was not carried out in the two-spatial dimensional case.

(2) Equation (2.1) is also equivalent to that presented in Ref. 18. The only difference is that the exponential of Eq. (5) of Ref. 18 involves $(x_l-\xi_l)/J_l^i$ instead of $(x_1-\xi_1)/J_1^i$ of (2.1). However, these two terms are equal due to the presence of the underlying δ functions.

(3) By letting $x_l\to x_l+J_l^i x_1/J_1^i$, $l=2,\ldots,n$, in Eq. (2.1) one may obtain a more symmetric equation for μ^{ij}:

$$\mu^{ij}\left(x_0,x_1,x_2+\frac{J_2^i}{J_1^i}x_1,\ldots,x_n+\frac{J_n^i}{J_1^i}x_1\right)$$
$$=\delta^{ij}+\tilde{g}^{ij}$$
$$\times(q\mu)^{ij}\left(\xi_0,\xi_1,x_2+\frac{J_2^i}{J_1^i}\xi_1,\ldots,x_n+\frac{J_n^i}{J_1^i}\xi_1,k\right), \tag{2.8}$$

where $\tilde{g}^{ij}$ is defined in (2.1).

(4) Equation (2.1) suggests that

$$\mu^{ij}(x_0,x,k)=\mu^{ij}\left(x_0,x_1,x_2-x_1\frac{J_2^i}{J_1^i},\ldots,x_n-x_1\frac{J_n^i}{J_1^i},k\right).$$

It also suggests that in the proper coordinate system, Eq. (1.3) should be reduced *locally* to one in only two dimensions. This is indeed the case: Equation (1.3) in component form becomes

$$\mu^{ij}_{x_0}+\sigma\sum_{l=1}^{n}J_l^i\mu^{ij}_{x_l}+i\sigma\sum_{l=1}^{n}k_l(J_l^i-J_l^j)\mu^{ij}=(q\mu)^{ij}. \tag{2.9}$$

Let

$$\Xi_0=x_0,\quad \Xi_1=x_1,\quad \Xi_r^i=x_r-x_1\frac{J_r^i}{J_1^i},\quad r=2,\ldots,n. \tag{2.10}$$

i.e.,

$$\frac{\partial}{\partial x_0}=\frac{\partial}{\partial\Xi_0},\quad \frac{\partial}{\partial x_r}=\frac{\partial}{\partial\Xi_r^i},\quad r=2,\ldots,n,$$
$$\frac{\partial}{\partial x_1}=\frac{\partial}{\partial\Xi_1}-\sum_{r=2}^{n}\frac{J_r^i}{J_1^i}\frac{\partial}{\partial\Xi_r^i}.$$

Then (2.9) yields

$$\mu^{ij}_{\Xi_0}+\sigma J_1^i\mu^{ij}_{\Xi_1}+i\sigma\sum_{l=1}^{n}k_l(J_l^i-J_l^j)\mu^{ij}=(q\mu)^{ij}. \tag{2.11}$$

(5) Equation (2.11), as well as Eq. (2.1) and (2.8), indicates that the direct problem associated with Eq. (1.3) is locally two dimensional. However, the two-spatial dimensional results of Ref. 8 are not directly applicable due to the shifting in the arguments. Let us illustrate this for the 2×2 case in three dimensions:

$$\mu^{11}(x_0,x_1,x_2,k)=1+\tilde{g}^{11}(q^1\mu^{21})(\xi_0,\xi_1,x_2-(x_1-\xi_1)J_2^1/J_1^1,k),$$
$$\mu^{21}(x_0,x_1,x_2,k)=\tilde{g}^{21}(q^2\mu^{11})(\xi_0,\xi_1,x_2-(x_1-\xi_1)J_2^2/J_1^2,k).$$

Clearly μ^{11} appears with different arguments in the two equations. However, one may still obtain a solution by iteration. The same is true for the equations corresponding to (2.8).

The next step is to relate $\partial\mu/\partial\bar{k}$ with μ. For this purpose the following proposition is important.

Proposition 2.2: (a) The function β^{ij} defined by (2.2) satisfies

$$\frac{\partial}{\partial\bar{k}_p}\exp[i\beta^{ij}(x_0,x_1,k)]=(\bar{\sigma}/2J_1^i\sigma_I)(x_1-x_0J_1^i)(J_p^i-J_p^j), \tag{2.12}$$

and

$$\beta^{ij}(k)-\beta^{ij}(k)=\beta^{ii}(k^{ij}(k)),$$
$$k_1^{ij}=\left[k_{1_R}-\sum_{l=1}^{n}\left(\frac{\sigma_R}{\sigma_I}k_{l_I}+k_{l_R}\right)\frac{J_l^i-J_l^j}{J_1^i},k_{1_I}\right], \tag{2.13}$$
$$k_r^{ij}=k_r,\quad r=2,\ldots,n.$$

In the above $\beta^{ij}(k)$ denotes $\beta^{ij}(x_0,x_1,k)$ and $k_1^{ij}=k_{1_R}^{ij}+ik_{1_I}^{ij}=[k_{1_R}^{ij},k_{1_I}^{ij}]$.

(b) The functions β^{ij} and α^i, defined by (2.2) and (2.4), respectively, satisfy

$$\alpha^l(m)+\beta^{lj}(k)-\alpha^i(M)-\beta^{ij}(k)=\alpha^l(m-M)+\beta^{li}(\lambda^{ij}(k,M)), \tag{2.14}$$

where

$$\lambda_1^{ij}=\left(k_{1_R}^{ij}-\sum_{l=2}^{n}M_l\frac{J_l^i}{J_1^i},k_{1_I}\right),$$
$$\lambda_r^{ij}=(k_{r_R}+M_r,k_{r_I}),\quad r=2,\ldots,n. \tag{2.15}$$

To derive Eq. (2.12) just use $\partial/\partial\bar{k}=\frac{1}{2}\partial/\partial k_R-(1/2i)\partial/\partial k_I$. To derive Eq. (2.13) note that

$$\beta^{lj}(k)-\beta^{ij}(k)=\sum_{r=1}^{n}\frac{1}{\sigma_I}\left[(J_r^l-J_r^i)x_0|\sigma|^2k_{r_I}-\left(\frac{J_r^l}{J_1^l}-\frac{J_r^i}{J_1^i}-\frac{J_r^i}{J_1^i}+\frac{J_r^j}{J_1^i}\right)x_1(\sigma k_r)_I\right].$$

But

$$\frac{J_r^l}{J_1^l}-\frac{J_r^j}{J_1^l}-\frac{J_r^i}{J_1^i}+\frac{J_r^j}{J_1^i}=\frac{J_r^l-J_r^i}{J_1^l}-\frac{(J_1^l-J_1^i)}{J_1^l}\frac{(J_r^i-J_r^j)}{J_1^i}. \tag{2.16}$$

Thus

$$\beta^{lj}(k)-\beta^{ij}(k)=\sum_{r=1}^{n}\frac{1}{\sigma_I}\left[(J_r^l-J_r^i)x_0|\sigma|^2k_{r_I}-\frac{(J_r^l-J_r^i)}{J_1^l}x_1(\sigma k_r)_I\right]+\frac{1}{\sigma_I}\frac{(J_1^l-J_1^i)}{J_1^l}x_1\times\sum_{r=1}^{n}\frac{(J_r^i-J_r^j)}{J_1^i}(\sigma k_r)_I.$$

Hence $\beta^{lj}(k)-\beta^{ij}(k)=\beta^{li}(k^{ij})$, where all the k's are invariant except k_1, which satisfies $k_{1_I}^{ij}=k_{1_I}$,

$$(\sigma k_1^{ij})_I=(\sigma k_1)_I-\sum_{r=1}^{n}(\sigma k_r)_I\frac{J_r^i-J_r^j}{J_1^i}.$$

To derive Eq. (2.14), note that its left-hand side equals

$$\sum_{r=2}^{n}(m_r-M_r)\left(x_r-x_1\frac{J_r^i}{J_1^i}\right)+\sum_{r=1}^{n}(J_r^l-J_r^i)\frac{x_0|\sigma|^2k_{r_I}}{\sigma_I}-\frac{(J_1^l-J_1^i)}{J_1^l}x_1\left[\sum_{r=2}^{n}-\frac{(J_r^i-J_r^j)}{J_1^i}\frac{(\sigma k_r)_I}{\sigma_I}+\frac{(\sigma k_1)_I}{\sigma_I}-\sum_{r=2}^{n}\frac{J_r^i}{J_1^i}M_r\right]-\sum_{r=2}^{n}\frac{J_r^l-J_r^i}{J_1^l}x_1\left[\frac{(\sigma k_r)_I}{\sigma_I}+M_r\right].$$

Hence, Eq. (2.14) follows, where λ^{ij} is defined by $\lambda_1^{ij}=k_1$

for all k's,

$$(\sigma\lambda^{ij}_r)_I = (\sigma k_r)_I + M_r, \quad r = 2,...,n,$$

$$(\sigma\lambda^{ij}_1)_I = (\sigma k^{ij}_1)_I - \sum_{r=2}^{n} M_r \frac{J^i_r}{J^i_1}.$$

Using the above relationships, $\partial\mu/\partial\bar{k}_p$, i.e., the departure from holomorphicity of the eigenfunction μ, can be evaluated in terms of μ and T.

Proposition 2.3: Let μ^{ij} be defined by Eq. (2.1). Then

$$\frac{\partial\mu}{\partial\bar{k}_p}(x_0,x,k) = \sum_{i,j} \gamma^j (J^i_p - J^j_p)\exp[i\beta^{ij}(x_0,x_1,k)] \times c_{n-1}\int_{\mathbf{R}^{n-1}} dm^2 \exp[i\alpha^i(x,m)] \times T^{ij}(k,m)\mu(x_0,x,\lambda^{ij}(k,m))E_{ij}, \tag{2.17}$$

where β^{ij}, α^i and λ^{ij} are defined by (2.2), (2.4), and (2.15), respectively; E_{ij} is an $N\times N$ matrix with zeros in all its entries except the ijth, which equals 1; and γ^j and T^{ij} are given by

$$\gamma^j \doteq \bar{\sigma}/4\pi i|J^i_1\sigma_I|,$$

$$T^{ij}(k,m) \doteq \int_{\mathbf{R}^{n+1}} d\xi_0\, d\xi \exp[-i\beta^{ij}(\xi_0,\xi_1,k) - i\alpha^i(\xi,m)](q\mu)^{ij}(\xi_0,\xi,k). \tag{2.18}$$

To derive Eq. (2.17) note that $\partial\mu^{ij}/\partial\bar{k}_p$ satisfies the same equation as μ^{ij}, where the forcing δ^{ij} is replaced by

$$c_{n-1}\gamma^j(J^i_p - J^j_p)\exp[i\beta^{ij}(x_0,x_1,k)] \times \int_{\mathbf{R}^{n-1}} dM^2 \exp[i\alpha^i(x,M)T^{ij}(k,M)].$$

Using $\mu = \Sigma_{i,j}\mu^{ij}E_{ij}$ it follows that the forcing of the equation satisfied by $\partial\mu/\partial\bar{k}_p$ is given by the above times E_{ij}. Hence

$$\frac{\partial\mu}{\partial\bar{k}_p} = \sum_{i,j}\gamma^j(J^i_p - J^j_p)c_{n-1} \times \int_{\mathbf{R}^{n-1}} dm^2\, T^{ij}(k,m)N_{ij}(x_0,x,k,m), \tag{2.19}$$

where N_{ij} is a matrix-valued function satisfying an equation similar to that of μ but with different forcing:

$$\text{if} \quad \mu(x_0,x,k) = I + (\tilde{G}\mu)(x_0,x,k),$$

$$\text{then} \quad N_{ij} = e^{i(\beta^{ij}+\alpha^i)}E_{ij} + \tilde{G}N_{ij}. \tag{2.20}$$

Equation (2.20) implies that $N_{ij} = (\mathbf{0},...,\mathbf{N}^j_{ij},...,\mathbf{0})$, where the components of the vector $\mathbf{N}^j_{ij}$ satisfy

$$N^{ij}_{ij}(x_0,x,k,M) = \exp[i(\beta^{ij}(x_0,x_1,k) + \alpha^i(x,M))]\delta^{ij} + (\tilde{G}^{ij}N^{ij}_{ij})(x_0,x,k,M). \tag{2.21}$$

Multiplying by the negative of the exponential appearing in (2.21) and using (2.14) it follows that $N^{ij}_{ij}(x_0,x,k,M) = \mu^{ij}(x_0,x,\lambda^{ij}(x,M))$. Hence

$$N_{ij} = [\underbrace{\mathbf{0},...,\mu^i(x_0,x,\lambda^{ij}),\mathbf{0},...,\mathbf{0}}_{j}] = \mu(x_0,x,\lambda^{ij})E_{ij}.$$

Using the above in (2.19) we obtain (2.17).

Proposition 2.4: The potential $q(x_0,x)$ of Eq. (1.3) can be reconstructed from

$$q(x_0,x) = \frac{i\sigma}{\pi}\hat{J}_p \int_{\mathbf{R}^2} dk'_{p_R}\, dk'_{p_I} \times \frac{\partial\mu}{\partial\bar{k}_p}(x_0,x,k_1,...,k_{p-1},k'_p,k_{p+1},...,k_n), \quad p = 1,...,n, \tag{2.22}$$

where $\partial\mu/\partial\bar{k}_p$ is evaluated by Eq. (2.17) in terms of T^{ij}, μ^{ij}. The eigenfunction μ is reconstructed by

$$\mu(x_0,x,k) = I + \frac{1}{\pi}\int_{\mathbf{R}^2} dk'_{p_R}\, dk'_{p_I} \times \frac{(\partial\mu/\partial\bar{k}_p)(x_0,x,k_1,...,k'_p,...,k_n)}{k_p - k'_p}, \quad p = 1,...,n. \tag{2.23}$$

To derive Eq. (2.23) invert $\bar{\partial}\mu$ in the variable k_p. To derive Eq. (2.22) note that if one seeks an asymptotic expansion of μ for large k_p in the form

$$\mu = I + \mu_1(x_0,x,k_1,...,k_{p-1},k_{p+1},...,k_n)/k_p + O(1/k^2_p),$$

one obtains, from (1.3), $q = i\sigma\hat{J}\mu_1$. This and large k_p asymptotics of (2.23) imply (2.22).

Remarks: (1) The forcing of the equation for $\partial\mu/\partial\bar{k}$ also can be written as

$$\sum_{i,j}\gamma^j(J^i_p - J^j_p)\exp[i\beta^{ij}(x_0,x_1,k)] \times t^{ij}(k;x_2 - x_1J^i_2/J^i_1,...,x_n - x_1J^i_n/J^i_1)E_{ij},$$

where

$$t^{ij} = c_{n-1}\int_{\mathbf{R}^{n-1}} dm^2 \exp[i\alpha^i(x,m)]T^{ij}(k,m).$$

(2) The results of Proposition (2.4) can be directly verified also (see below).

III. ON AN IMPLICIT CHARACTERIZATION

Equation (2.23) indicates that there exist n inversion formulas for μ. Furthermore Eq. (2.22) indicates that, unless the inverse data T^{ij} are appropriately constrained, the reconstructed q will depend on k. We now show explicitly that q being independent of k is equivalent to the equality of all the inversion formulas. This is a direct consequence of the following result.

Proposition 3.1: Let us define the operators $L_k, F_{x_0,x,k-k_p}$ by

$$(L_k g)(x_0,x) \doteq \frac{\partial g}{\partial x_0} + \sigma\sum_{l=1}^{n} J_l\frac{\partial g}{\partial x_l} + i\sigma\sum_{l=1}^{n} k_l[J_l,g], \tag{3.1}$$

$$(F_{x_0,x,k-k_p}\, g)(k_p)$$

$$\doteq \frac{1}{\pi}\int_{\mathbf{R}^2} dk'_{p_R}\, dk'_{I_R}$$

$$\times \frac{\Sigma_{i,j}\gamma^i(J^i_p - J^j_p)c_{n-1}\int_{\mathbf{R}^{n-1}} dm^2 \exp[i\epsilon^{ij}(x_0,x,k^{p'},m)]\, T^{ij}(k^{p'},m)\, g(x_0,x,\lambda^{ij}(k^{p'},m))E_{ij}}{k_p - k'_p}, \tag{3.2}$$

where

$$\epsilon^{ij}(x_0,x,k,m) \doteq \beta^{ij}(x_0,x_1,k) + \alpha^i(x,m), \quad k^{p'} \text{ denotes } k_1,k_2,\ldots,k'_p,\ldots,k_n. \tag{3.3}$$

We use $F_{x_0,x,k-k_p}$ to denote that F depends on x_0,x,k_l, $l=1,\ldots,n$, $l\neq p$. Then

$$[L_k, F_{x_0,x,k-k_p}]\, g(x_0,x,k)$$

$$= \frac{i\sigma}{\pi}\hat{J}_p \int_{\mathbf{R}^2} dk'_{p_R}\, dk'_{p_I} \sum_{i,j}\gamma^i(J^i_p - J^j_p)c_{n-1}\int_{\mathbf{R}^{n-1}} dm^2 \exp[i\epsilon^{ij}(x_0,x,k^{p'},m)]\, T^{ij}(k^{p'},m)\, g(x_0,x,\lambda^{ij}(k^{p'},m))E_{ij}. \tag{3.4}$$

To derive Eq. (3.4) note that the term $L_k(F_{x_0,x,k-k_p}\, g)$ involves

$$\left[i\left(\frac{\partial}{\partial x_0} + \sigma\sum_{l=1}^n J_l\frac{\partial}{\partial x_l}\right)\epsilon^{ij}(k^{p'})\right] gE_{ij} + \left(-\frac{\partial}{\partial x_0} + \sigma\sum_{l=1}^n J_l\frac{\partial}{\partial x_l}\right) gE_{ij} + i\sigma\sum_{l=1}^n k_l[J_l, gE_{ij}],$$

while the term $F_{x_0,x,k-k_p}(L_k\, g)$ involves

$$\left(\frac{\partial}{\partial x_0} + \sigma\sum_{l=1}^n J_l\frac{\partial}{\partial x_l}\right) gE_{ij} + i\sigma\sum_{l=1}^n \lambda^{ij}_l(k^{p'})[J_l, g]E_{ij}.$$

Two of the above expressions cancel out, also, since $(gE_{ij})^{rf}$ is nonzero only if $j=f$, in which case it equals g^{ri},

$$\left\{\left[\left(\frac{\partial}{\partial x_0} + \sigma\sum_{l=1}^n J_l\frac{\partial}{\partial x_l}\right)\epsilon^{ij}\right] gE_{ij}\right\}^{rf} = \left\{\left[\left(\frac{\partial}{\partial x_0} + \sigma\sum_{l=1}^n J_l\frac{\partial}{\partial x_l}\right)\epsilon^{ij}\right] g\right\}^{ri} = \left[\left(\frac{\partial}{\partial x_0} + \sigma\sum_{l=1}^n J^r_l\right)\epsilon^{ij}\right] g^{ri},$$

$$[J_l, gE_{ij}]^{rf} = (J^r_l - J^f_l)(gE_{ij})^{rf} = (J^r_l - J^f_l)\, g^{ri}, \quad \{[J_l,g]E_{ij}\}^{rf} = [J_l,g]^{ri} = (J^r_l - J^i_l)\, g^{ri}.$$

Hence, $[L_k, F_{x_0,x,k-k_p}]\, g$ involves $i\sigma g^{ri}$ times

$$\sum_{l=1}^n k_l(J^r_l - J^f_l) + \sum_{l=1}^n \frac{J^i_l - J^j_l}{\sigma_I}\bar{\sigma}k^{p'}_{l_I} - J^r_1\sum_{l=1}^n \frac{J^i_l - J^j_l}{J^i_l}\left(k^{p'}_{l_R} + \frac{\sigma_R}{\sigma_I}k^{p'}_{l_I}\right) - J^r_1\sum_{l=2}^n m_l\frac{J^i_l}{J^i_1} + \sum_{l=2}^n J^r_l m_l$$

$$- \sum_{l=2}^n (J^r_l - J^i_l)(ik^{p'}_{l_I} + k^{p'}_{l_R} + m_l) - (J^r_1 - J^i_1)\left[ik^{p'}_{1_I} + k^{p'}_{1_R} - \sum_{l=1}^n\left(k^{p'}_{l_R} + \frac{\sigma_R}{\sigma_I}k^{p'}_{l_I}\right)\frac{J^i_l - J^j_l}{J^i_1} - \sum_{l=2}^n\frac{J^i_l}{J^i_1}m_l\right].$$

The above expression equals

$$\sum_{l=1}^n k_l(J^r_l - J^f_l) - \sum_{l=1}^n k^{p'}_l(J^r_l - J^f_l) = (k_p - k'_p)(J^r_p - J^f_p),$$

which implies Eq. (3.4).

Remarks: (1) The above proposition implies that the direct linearizing method[20,21] is also valid here. The relevant result is directly analogous to that of the two-dimensional case.[9]

(2) $q = [L_k, F_{x_0,x,k-k_p}]\,\mu$, $p=1,\ldots,n$, where the pth expression is independent of k_p. Suppose that q is independent of k_p,k_r, then $[L_k, F_{x_0,x,k-k_p}]\,\mu = [L_k, F_{x_0,x,k-k_r}]\,\mu$. Hence $(F_{x_0,x,k-k_p})\,\mu = (F_{x_0,x,k-k_r})\,\mu$, i.e., the pth and the rth inversion formulas are equal. Similarly, if the pth and the rth inversion formulas are equal, q is independent of both k_p and k_r.

IV. ON AN EXPLICIT CHARACTERIZATION

Proposition 4.1: (a) Assume that $\partial\mu/\partial\bar{k}_p$ is given by Eq. (2.17) and that $T^{ij}(k,m)$ is given by (2.18). Then

$$L^{ij}_{rp}T^{ij}(k,m) = -\sum_{l=1}^n c_{n-1}\int_{\mathbf{R}^{n-1}} dM^2\, T^{il}(\lambda^{ij}(k,M),m-M)T^{lj}(k,m)$$

$$\times[(J^l_p - J^j_p)(J^i_r - J^l_r) - (J^l_r - J^j_r)(J^i_p - J^l_p)] \doteq N^{ij}_{rp}[T](k,m), \tag{4.1}$$

where

$$L^{ij}_{rp} \doteq (J^i_p - J^j_p)\frac{\partial}{\partial\bar{k}_r} - (J^i_r - J^j_r)\frac{\partial}{\partial\bar{k}_p}. \tag{4.2}$$

(b) Assume that $\partial\mu/\partial\bar{k}_p$ is given by Eq. (2.17) and that $\partial^2\mu/\partial\bar{k}_r\,\partial\bar{k}_p$ is symmetric with respect to r,p. Then $T^{ij}(k,m)$ solves (4.1).

To derive Eq. (4.1) note that

$$L^{ij}_{rp}T^{ij}=\int_{\mathbb{R}^{n+1}}d\xi_0\,d\xi_1\exp[-i\epsilon^{ij}(\xi_0,\xi,k,m)]\left\{q\left[(J^i_p-J^j_p)\frac{\partial\mu(k)}{\partial\bar{k}_r}-(J^i_r-J^j_r)\frac{\partial\mu(k)}{\partial\bar{k}_p}\right]\right\}^{ij}$$

$$=c_{n-1}\int_{\mathbb{R}^{n+1}}d\xi_0\,d\xi_1\exp[-i\epsilon^{ij}(\xi_0,\xi,k,m)]\left\{\int_{\mathbb{R}^{n-1}}dM^2\sum_{l,f}\gamma^f\exp[ie^{if}(\xi_0,\xi,k,m)]\right.$$

$$\left.\times T^{if}(k,M)[(J^i_p-J^j_p)(J^l_r-J^f_r)-(J^i_r-J^j_r)(J^l_p-J^f_p)](q\mu)(\lambda^{if}(k,M))E_{lf}\right\}^{ij}.$$

Since $(\mu E_{lf})^{ij}$ is nonzero only if $j=j'$, evaluate the above at $j=j'$. Also, Eq. (2.14) implies $-\epsilon^{if}(k,M)+\epsilon^{lf}(k,M)=-\beta^{il}(\lambda^{if}(k,M))-\alpha^l(m-M)$, and, since

$$\int_{\mathbb{R}^{n+1}}d\xi_0\,d\xi_1\exp[-i\beta^{if}(\lambda^{if}(k,M))]\exp[-i\alpha^l(m-M)](q\mu)^{li}(\lambda^{if}(k,M))=T^{li}(\lambda^{if}(k,M),m-M),$$

Eq. (4.1) follows.

To derive the second statement of Proposition (4.1) first note

$$L^{ij}_{rp}e^{i\beta^{ij}}(k)=0,\quad L^{ij}_{rp}\mu(\lambda^{ij}(k,m))=L^{ij}_{rp}\mu(K),\tag{4.3}$$

$$\beta^{ij}(k)+\alpha^i(m)+\beta^{ri}(\lambda^{ij}(k,m))+\alpha^r(M)=\beta^{rj}(k)+\alpha^r(M+m),\quad \lambda^{ri}(\lambda^{ij}(k,m),M)=\lambda^{rj}(k,m+M).\tag{4.4}$$

Equation (4.3a) follows from (2.12). Equation (4.3b) means that, with respect to the operator $L_{r,p}$, $\mu(\lambda^{ij})$ should be treated as if its k's were not shifted; it is an obvious consequence of the definition of λ^{ij}. To derive Eq. (4.4a) use (2.14) to substitute for

$$\beta^{ri}(\lambda^{ij}(k,m))=\alpha^r(M)+\beta^{rj}(k)-\alpha^i(m)-\beta^{ij}(k)-\alpha^r(M-m).$$

Equation (4.4b) follows from the definition of λ^{ij}:

$$\lambda^{ij}_{1_R}(k,m)=k_{1_R}\frac{J^j_1}{J^i_1}-\frac{\sigma_R}{\sigma_I}k_{1_I}\frac{(J^i_1-J^j_1)}{J^i_1}-\sum_{l=2}^{n}\left(k_{l_R}+\frac{\sigma_R}{\sigma_I}k_{l_I}\right)\frac{J^i_1-J^j_1}{J^i_1}-\sum_{l=2}^{n}m_l\frac{J^i_l}{J^i_1}.$$

Hence,

$$\lambda^{ri}_{1_R}(\lambda^{ij}(k,m),M)=\frac{J^i_1}{J^r_1}\left\{k_{1_R}\frac{J^j_1}{J^i_1}-\frac{\sigma_R}{\sigma_I}k_{1_I}\left(\frac{J^i_1-J^j_1}{J^i_1}\right)-\sum_{l=2}^{n}\left(k_{l_R}+\frac{\sigma_R}{\sigma_I}k_{l_I}\right)\frac{(J^i_l-J^j_l)}{J^i_1}-\sum_{l=2}^{n}m_l\frac{J^i_l}{J^i_1}\right\}$$

$$-\frac{\sigma_R}{\sigma_I}k_{1_I}\left(\frac{J^r_1-J^i_1}{J^r_1}\right)-\sum_{l=2}^{n}\left(k_{l_R}+m_l+\frac{\sigma_R}{\sigma_I}k_{l_I}\right)\left(\frac{J^r_l-J^i_l}{J^r_1}\right)-\sum_{l=2}^{n}M_l\frac{J^r_l}{J^r_1}$$

$$=k_{1_R}\frac{J^j_1}{J^r_1}-\frac{\sigma_R}{\sigma_I}k_{1_I}\left(\frac{J^r_1-J^j_1}{J^r_1}\right)-\sum_{l=2}^{n}\left(k_{l_R}+\frac{\sigma_R}{\sigma_I}k_{l_I}\right)\left(\frac{J^r_l-J^j_l}{J^r_1}\right)-\sum_{l=2}^{n}(m_l+M_l)\frac{J^r_l}{J^r_1}=\lambda^{rj}_{1_R}.$$

Let

$$\Delta\mu\doteq\frac{\partial^2\mu}{\partial\bar{k}_r\,\partial\bar{k}_p}-\frac{\partial^2\mu}{\partial\bar{k}_p\,\partial\bar{k}_r}=c_{n-1}\sum_{i,j}\int_{\mathbb{R}^{n-1}}dm^2\,\gamma^jL^{ij}_{rp}\{e^{i\epsilon^{ij}}(k,m)T^{ij}(k,m)\,\mu(\lambda^{ij})E^{ij}\}.$$

Using (4.3) it follows that

$$\Delta\mu=c_{n-1}\sum_{i,j}\int_{\mathbb{R}^{n-1}}dm^2\,\gamma^j\exp[i\epsilon^{ij}(k,m)](L^{ij}_{rp}T^{ij})\,\mu(\lambda^{ij})E^{ij}$$

$$+c_{2n-2}\sum_{i,j,i',j}\int_{\mathbb{R}^{2n-2}}dm^2\,dM^2\,\gamma^j\gamma^{j'}\exp\{i[\epsilon^{ij}(k,m)+\epsilon^{i'j'}(\lambda^{ij}(k,m),M)]\}T^{ij}(k,m)T^{i'j'}(\lambda^{ij}(k,m),M)$$

$$+c_{2n-2}\sum_{i,j,i',j}\int_{\mathbb{R}^{2n-2}}dm^2\,dM^2\,\gamma^j\gamma^{j'}\exp\{i[\epsilon^{ij}(k,m)+\epsilon^{i'j'}(\lambda^{ij}(k,m),M)]\}$$

$$\times T^{ij}(k,m)T^{i'j'}(\lambda^{ij}(k,m),M)\pi\mu(\lambda^{i'j'}(\lambda^{ij}(k,m),M)E_{i'j'}E_{ij},$$

where $\pi\doteq(J^i_p-J^j_p)(J^{i'}_r-J^{j'}_r)-(J^i_r-J^j_r)(J^{i'}_p-J^{j'}_p)$. Since $E_{i'j'}E_{ij}$ is nonzero only if $i=j'$, in which case it equals E_{ij}, it follows that the above should be investigated at $i=j'$. Then the first term of $\Delta\mu$ involves $\int dp\,\gamma^j\exp[i\epsilon^{ij}(k,p)](L^{ij}_{rp}T^{ij}(k,p))\mu(\lambda^{ij}(k,p))$, while the second term involves [using Eq. (4.4) and letting $m+M=p$]

$$\int_{\mathbb{R}^2}dp\,dm\,\gamma^i\gamma^j\exp[i\epsilon^{ij}(k,p)]T^{ij}(m)T^{ri}(\lambda^{ij}(k,m),p-m)\mu(\lambda^{rj}(k,p)).$$

Thus $\Delta\mu=0$ implies the "T-equation" (4.1) [to obtain the identical variables of (4.1), let $i'\to i$, $i\to l$, $p\to m$, $m\to M$].

We now derive an equation providing an explicit characterization for the inverse data T.

Proposition 4.2: Let w^{ij}_0,w^{ij}_1,w_l, $l=2,\ldots,n\in\mathbb{R}^1$ and $\chi_l\in\mathbb{C}^1$, $l=2,\ldots,n$, be defined by

$$w_0^{ij} \doteq \sum_{r=1}^{n} \frac{J_r^i - J_r^j}{\sigma_I} |\sigma|^2 k_{r_I}, \quad w_1^{ij} \doteq -\sum_{r=1}^{n} \frac{J_r^i - J_r^j}{\sigma_I J_1^i} (\sigma k_r)_I - \sum_{r=2}^{n} m_r \frac{J_r^i}{J_1^i}, \quad w_l \doteq m_l, \quad \chi_l^{ij} \doteq \frac{k_l}{J_1^j - J_1^i}, \quad l = 2,...,n. \tag{4.5}$$

Assume that

$$(J_1^r - J_1^j)(J_p^i - J_p^j) \neq (J_1^i - J_1^j)(J_p^r - J_p^j), \quad \text{for all distinct } i,j,r \text{ and } p \neq 1. \tag{4.6}$$

For convenience of writing we usually suppress the superscripts i,j in w_0, w_1, χ. Let k denote $k_1,...,k_n$, m denote $m_2,...,m_n$, χ denote $\chi_2,...,\chi_n$, w denote $w_1,...,w_n$. Then we have the following.

(a) The inverse of the transformation $k,m \to w_0,w,\chi$ is given by

$$k_l = \chi_l (J_1^j - J_1^i), \quad m_l = w_l, \quad l = 2,...,n, \quad k_1 = -\sum_{r=2}^{n} (J_r^j - J_r^i)\chi_r + \frac{(\bar{\sigma}/|\sigma|^2) w_0 + \Sigma_{r=1}^{n} w_r J_r^i}{J_1^j - J_1^i}. \tag{4.7}$$

(b) In the new coordinates, Eq. (4.1) with $r = 1$ becomes

$$\frac{\partial T^{ij}}{\partial \bar{\chi}_p}(w_0,w,\chi) = N_{1p}^{ij}[T](w_0,w,\chi), \quad p = 2,...,n. \tag{4.8}$$

(c) In the new coordinates

$$T^{ij}(w_0,w,\chi) = \int_{\mathbf{R}^{n+1}} d\xi_0\, d\xi \exp[-i(w_0\xi_0 + w\xi)](q\mu)^{ij}(\xi_0,\xi,w_0,w,\chi), \quad \text{where} \quad w\xi = \sum_{r=1}^{n} w_r \xi_r. \tag{4.9}$$

(d) Let

$$\mu_l^{ij} \doteq \mu^{ij}(x_0,x,w_0^{ij},w^{ij},\chi^{ij}), \quad \hat{\mu}_l^{ij} = \lim_{|\chi_p| \to \infty} \mu_l^{ij}. \tag{4.10}$$

Then the $\hat{\mu}_l^{ij}$ satisfy

$$\hat{\mu}_i^{ij}(x_0,x,w_0,w) = \operatorname{sgn}\frac{(\sigma_I J_1^i)}{2\pi i} c_{n-1} \int_{\mathbf{R}^{2n}} \frac{dx_0'\, dx'\, dm^2 \exp[i\{(x_0 - x_0')w_0 + (x - x')w\}]}{x_1 - x_1' - \sigma J_1^i (x_0 - x_0')} q^{ij}(x_0',x')\, \hat{\mu}_i^{jj}(x_0',x',w_0,w),$$

$$\hat{\mu}_i^{jj}(x_0,x,w_0,w) = 1 + \frac{\operatorname{sgn}(\sigma_I J_1^j)}{2\pi i} c_{n-1} \int_{\mathbf{R}^{2n}} \frac{dx_0'\, dx'\, dm^2\, q^{ji}(x_0',x')\, \hat{\mu}_i^{ij}(x_0',x',w_0,w)}{x_1 - x_1' - \sigma J_1^j (x_0 - x_0')}, \quad \hat{\mu}_l^{ij} = 0, \quad \text{for all } l, \ l \neq i, \ l \neq j. \tag{4.11}$$

(e) $$\lim_{|\chi_p| \to \infty} T^{ij}(w_0,w,\chi) = \int_{\mathbf{R}^{n+1}} d\xi_0\, d\xi \exp[-i(w_0\xi_0 + w\xi)] q^{ij}(\xi_0,\xi)\, \hat{\mu}_i^{jj}(\xi_0,\xi,w_0,w) \doteq \hat{T}^{ij}(w_0,w). \tag{4.12}$$

(f) The basic characterization equation is given by

$$\hat{T}^{ij}(w_0,w) = T^{ij}(w_0,w,\chi) - \frac{1}{\pi} \int_{\mathbf{R}^2} \frac{d\chi_{p_R}'\, d\chi_{p_I}'\, N_{1p}^{ij}[T](w_0,w,\chi^{p'})}{\chi_p - \chi_p'}. \tag{4.13}$$

where $\chi^{p'}$ denotes $\chi_2,...,\chi_{p-1},\chi_p',\chi_{p+1},...,\chi_n$.

The transformation $k,m \to w_0,w,\chi$ is motivated by the following requirements:

$$\beta^{ij}(x_0,x_1,k) + \alpha^i(x,m) = w_0 x_0 + wx, \quad L_{1p}^{ij} = \frac{\partial}{\partial \bar{\chi}_p}. \tag{4.14}$$

Equations (4.14) also imply (a)–(c) above. To derive (d) of Proposition 4.2, note that T^{ij} depends on μ^{ij}. Thus in order to compute $\hat{T}^{ij}(w_0,w)$, one needs $\mu^{ij}(x_0,x,w_0^{ij},w^{ij},\chi^{ij})$ for large χ_p^{ij}. The eigenfunction μ^{ij} satisfies (2.3), hence the relevant exponential will involve $\beta^{ij} + \alpha^l$ in the new coordinates:

$$\beta^{ij}(x_0,x_1,w_0,w,\chi) + \alpha^l(x,w) = \sum_{r=2}^{n} w_r \left\{ x_r - \left[\frac{J_1^j (J_r^l - J_r^i) + J_r^i J_1^l - J_r^l J_1^i}{J_1^l (J_1^j - J_1^i)} \right] x_1 \right\} - \frac{J_1^l - J_1^j}{J_1^j - J_1^i} \left(x_0 w_0 + x_1 w_1 \frac{J_1^i}{J_1^l} \right)$$
$$+ \sum_{r=2}^{n} \epsilon_r^{lji} \left[x_0 \frac{|\sigma|^2}{\sigma_I} \chi_{r_I} - \frac{x_1}{\sigma_I J_1^l} (\sigma \chi_r)_I \right], \tag{4.15}$$

where

$$\epsilon_r^{lji} \doteq (J_1^l - J_1^i)(J_r^l - J_r^j) - (J_r^j - J_r^i)(J_1^l - J_1^j). \tag{4.16}$$

As $|\chi| \to \infty$ the relevant exponential tends to zero unless $\epsilon_p^{lji} = 0$, which occurs for $l = j$ and $l = i$. Hence, one is left with only two nonzero contributions: For $l = j$, in which case $\beta^{jj} + \alpha^j = 0$, and for $l = i$ in which case $\beta^{ij} + \alpha^i = x_0 w_0 + wx$. Thus $\hat{\mu}_i^{ij}$ satisfy Eq. (4.11). Equation (4.12) follows from (4.9), (4.11), and the fact that $q^{ii} = 0$. To obtain (4.13) just invert $\bar{\partial}$ and use (4.12).

Remarks: (1) Equation (4.12) can be thought of as the

analog of the Born approximation of the Schrödinger equation. However, because $\epsilon_p^{jjl}=0$, one does not simply obtain the Fourier transform of q^{ij}.

(2) Suppose that the J_l's are constrained via

$$\frac{J_p^l-J_p^j}{J_r^l-J_r^j}=\frac{J_p^i-J_p^j}{J_r^i-J_r^j},$$
$$p,r=1,\ldots,n,\quad i,j,l=1,\ldots,N. \tag{4.17}$$

Then the assumption (4.6) is violated and the above procedure fails. However, in this case the whole problem of characterization may be bypassed: Both Eqs. (1.3) and (2.1) indicate that one may introduce a single parameter $\hat{k}$, which is a combination of the k_l's iff

$$\sum_1^n (J_l^i-J_l^j)k_l=(J_1^i-J_1^j)\hat{k},\quad \text{for all } i,j=1,\ldots,N. \tag{4.18}$$

If $N=2$, or if Eqs. (4.17) are valid, then the solution $\hat{k}$ of Eqs. (4.18) always exists. To fix ideas, consider $N=3$. Then Eqs. (4.18) are solvable iff

$$\frac{\Sigma_1^n(J_l^1-J_l^2)k_l}{J_1^1-J_1^2}=\frac{\Sigma_1^n(J_l^1-J_l^3)k_l}{J_1^1-J_1^3}=\frac{\Sigma_1^n(J_l^2-J_l^3)k_l}{J_1^2-J_1^3}. \tag{4.19}$$

However, if Eqs. (4.17) are valid then

$$\frac{J_l^1-J_l^2}{J_1^1-J_1^2}=\frac{J_l^1-J_l^3}{J_1^1-J_1^3}=\frac{J_l^2-J_l^3}{J_1^2-J_1^3}.$$

Multiplying the above by k_l and summing over l we obtain (4.19). The general N case is a trivial extension of the above, where one uses

$$(J_l^i-J_l^j)/(J_1^i-J_1^j)=(J_l^i-J_l^j)/(J_1^i-J_1^j).$$

(3) Remark (2) implies that if $N=2$ or if the J_l's satisfy (4.17) then one can always introduce a single $\hat{k}$. Hence, the eigenvalue problems associated with these cases should be reducible to two dimensions. This fact is used below since the reduced system (4.11a) and (4.11b) corresponds to $N=2$.

(4) The N-wave interaction equations are associated with (1.3) when $\sigma=-1$ and the J_l's satisfy (4.19). Therefore, it is not surprising that these equations always can be reduced to two dimensions.[19]

V. THE RECONSTRUCTION OF q

We now present a more efficient way of reconstructing q than that of Sec. II. Equations (4.11a) and (4.11b) define a system of two equations for the eigenfunctions $\hat{\mu}_l^{ij},\hat{\mu}_l^{jj}$ in terms of the 2×2 matrix potential with entries q^{ij},q^{ji}. We consider the inverse problem associated with this system: what are the necessary inverse data needed for the reconstruction of q^{ij},q^{ji}? In what follows we show that (a) one can always introduce a new, single $\hat{k}\in\mathbb{C}^1$ [this is consistent with Remark (3) above, since in this case $N=2$]; (b) with a proper change of variables, the above system can be reduced to two dimensions; and (c) the inverse data needed for the solution of this problem is simply related to $\hat{T}^{ij},\hat{T}^{ji}$.

Proposition 5.1: Let

$$\alpha_r\doteq\frac{J_2^jJ_r^i-J_r^jJ_2^i}{J_1^iJ_2^j-J_1^jJ_2^i},$$
$$\beta_r=\frac{J_1^iJ_r^j-J_1^jJ_r^i}{J_1^iJ_2^j-J_1^jJ_2^i},\quad r=1,\ldots,n, \tag{5.1}$$

where for convenience of writing we have suppressed the dependence of α_r,β_r on i,j. Let $\xi_0\in\mathbb{R}$, $\xi\in\mathbb{R}^n$,

$$x_0=\xi_0,\quad x_1=\xi_1,\quad x_2=\xi_2,$$
$$x_l=\xi_l+\alpha_l\xi_1+\beta_l\xi_2,\quad l=3,\ldots,n. \tag{5.2}$$

Then we have the following.

(a) The system (4.11a) and (4.11b) becomes

$$\begin{aligned}\hat{\mu}_l^{ij}(\xi_0,\xi,\hat{k})=\operatorname{sgn}\frac{\sigma_IJ_1^i}{2\pi i}\int_{\mathbb{R}^2}d\xi_0'\,d\xi_1'\\ \times[\xi_1-\xi_1'-\sigma J_1^i(\xi_0-\xi_0')]^{-1}\\ \times\exp[i\hat{\beta}^{ij}(\xi_0-\xi_0',\xi_1-\xi_1',\hat{k})]\\ \times q^{ij}\hat{\mu}_l^{jj}(\xi_0',\xi_1',\xi_2\\ -(\xi_1-\xi_1')J_2^i/J_1^i,\xi_3,\ldots,\xi_n,\hat{k}),\end{aligned}$$

$$\begin{aligned}\hat{\mu}_l^{jj}(\xi_0,\xi,\hat{k})\\ =1+\operatorname{sgn}\frac{\sigma_IJ_1^j}{2\pi i}\int_{\mathbb{R}^2}d\xi_0'\,d\xi_1'\\ \times[\xi_1-\xi_1'-\sigma J_1^j(\xi_0-\xi_0')]^{-1}\\ \times q^{ji}\hat{\mu}_l^{ij}(\xi_0',\xi_1',\xi_2\\ -(\xi_1-\xi_1')J_2^j/J_1^j,\xi_3,\ldots,\xi_n,\hat{k}),\end{aligned} \tag{5.3}$$

where

$$\begin{aligned}\hat{k}\doteq\sum_{r=1}^n\left(k_r\alpha_r+\frac{J_2^j-J_2^i}{J_1^j-J_1^i}k_r\beta_r\right)\hat{\beta}^{ij}(x_0,x_1,\hat{k})\\ \doteq\frac{J_1^i-J_1^j}{\sigma_I}\left[x_0|\sigma|^2k_I-x_1\frac{(\sigma k)_I}{J_1^i}\right].\end{aligned} \tag{5.4}$$

(b) $\hat{T}^{ij}$ in the new coordinates becomes

$$\begin{aligned}\hat{T}^{ij}(\hat{k},\hat{m})=\int_{\mathbb{R}^{n+1}}d\xi_0'\,d\xi'\exp\Big[-i\hat{\beta}^{ij}(\xi_0',\xi_1',\hat{k})\\ +\hat{m}_2\Big(\xi_2'-\xi_1'\frac{J_2^i}{J_1^i}\Big)+\sum_{r=3}^n\hat{m}_r\xi_r'\Big]\\ \times\hat{q}^{ij}\hat{\mu}_l^{jj}(\xi_0',\xi',\hat{k}),\end{aligned} \tag{5.5}$$

where

$$\hat{m}_2\doteq m_2+\sum_{r=3}^n m_r\beta_r,\quad \hat{m}_l=m_l,\quad l=3,\ldots,n. \tag{5.6}$$

(c) The inverse data associated with (5.3) and the analogous problem for $\hat{\mu}_j^{ji}$, $\hat{\mu}_j^{ij}$ are given by $\tilde{T}^{ij},\tilde{T}^{ji}$. Let

$$\begin{aligned}\tilde{T}^{ij}(k,\xi_2-\xi_1J_2^i/J_1^i,\xi_3,\ldots,\xi_n)\\ \doteq c_{n-1}\int_{\mathbb{R}^{n-1}}d\hat{m}\exp\Big[i\hat{m}_2\Big(\xi_2-\xi_1\frac{J_2^i}{J_1^i}\Big)\\ +i\sum_{r=3}^n\hat{m}_r\xi_r\Big]\hat{T}^{ij}(\hat{k},\hat{m}).\end{aligned} \tag{5.7}$$

Then

$$\tilde{T}^{ij}(\hat{k},\xi_2-\xi_1 J_2^i/J_1^i,\xi_3,\ldots,\xi_n)$$
$$\doteq\int_{\mathbb{R}^2} d\xi_0'\,d\xi_1'\,\exp[-i\hat{\beta}^{ij}(\xi_0',\xi_1',\hat{k})]$$
$$\times(q^{ij}\hat{\mu}_i^{jj})(\xi_0',\xi_1',\xi_2$$
$$-(\xi_1-\xi_1')J_2^i/J_1^i,\xi_3,\ldots,\xi_n,\hat{k}). \tag{5.8}$$

To derive the above results note that the definitions (5.1) and (5.4a) are motivated from the fact that we are now dealing only with two equations:

$$\hat{\mu}^{ij}_{i_{x_0}}+\sigma\sum_{l=1}^{n}\{J_l^i\hat{\mu}^{ij}_{i_{x_l}}+ik_l(J_l^i-J_l^j)\hat{\mu}_i^{ij}\}=q^{ij}\hat{\mu}_i^{jj},$$
$$\hat{\mu}^{jj}_{i_{x_0}}+\sigma\sum_{l=1}^{n}J_l^j\mu^{jj}_{i_{x_l}}=q^{ji}\hat{\mu}_i^{ij}. \tag{5.9}$$

Hence all the J_l's are linearly related and furthermore one can introduce a new $\hat{k}$ [see Remark (3) above]:

$$J_r^i=\alpha_r J_1^i+\beta_r J_2^i,\quad J_r^j=\alpha_r J_1^j+\beta_r J_2^j,$$
$$\hat{k}(J_1^i-J_1^j)\doteq\sum_{r=1}^{n}(J_r^i-J_r^j)k_r. \tag{5.10}$$

Substituting (5.10a) and (5.10b) in (5.9) we are motivated to introduce new variables ξ_0,ξ.

To derive (a) from (4.11) we calculate $(x_0-x_0')w_0+(x-x')w$ in the new coordinates:

$$w_0x_0+wx=\hat{\beta}^{ij}(\xi_0,\xi_1,\hat{k})$$
$$+\hat{m}_2\left(\xi_2-\xi_1\frac{J_2^i}{J_1^i}\right)+\sum_{r=3}^{n}m_r\xi_r. \tag{5.11}$$

Hence Eqs. (4.11) imply (5.3), since both Jacobians from (x_0,x) to (ξ_0,ξ) and from m to $\hat{m}$ are equal to unity.

Equations (5.10) and (4.9) imply (5.5). Multiplying Eq. (5.5) by

$$c_{n-1}\exp[i\hat{m}_2(\xi_2-\xi_1J_2^i/J_1^i)+i\Sigma_{r=3}^{n}\hat{m}_r\xi_r]$$

and integrating over $\mathbb{R}^{n-1}$ we obtain that $\tilde{T}^{ij}$ satisfies (5.8). However, the inverse data $\tilde{T}^{ij}$ and the analogous $\tilde{T}^{ji}$ are precisely what is needed for solving the inverse problem associated with (5.3) and the analogous equations obtained by interchanging i and j.

Remarks: (1) The above results are consistent with the fact that, in the coordinates (5.2), Eqs. (5.9) reduce to two dimensions.

(2) The two-dimensional problem is solved in Ref. 8.

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A class of solvable second-order ordinary differential equations with variable coefficients

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This paper treats the problem of solving the second-order ordinary differential equations with variable coefficients of the form $d^2x/dt^2 + [q_1(t) + \lambda q_2(t)]x = 0$. It is shown that if the initial equation $d^2x/dt^2 + q_1(t)x = 0$ is in analytically solvable form and $q_2(t)$ is the inverse square function of a solution for the nonlinear auxiliary equation $\frac{1}{2}x\,d^2x/dt^2 - \frac{1}{4}(dx/dt)^2 + q_1(t)x^2 = 1$, there are exact solutions. Using an inner relationship between solutions for the initial equation and the auxiliary equation, an infinite sequence of analytically solvable differential equations is constructed step by step. Typical examples of such a sequence are shown.

I. INTRODUCTION

Most physical problems exhibit certain essential features that seem to preclude exact analytical solutions at first glance. Some of these features are second-order ordinary differential equations with variable coefficients. In order to obtain information about solutions of such equations, we are usually forced to resort to approximations, numerical solutions, or combinations of both. Each has disadvantages; for instance, effectiveness of perturbation methods (approximations) is restricted to the case where a small or large parameter appears in equations. Meanwhile, numerically solving equations is time consuming, and obtained results scarcely indicate clear dependences of them on parameters involved in an equation.

It is most desirable to derive analytical solutions; however, this struggle for solutions is usually too exhaustive. If, before approaching a solution, it is realized whether or not the equations in question have exact analytical solutions, one can avoid unnecessary work. To the author's knowledge, there are no general methods to distinguish between the two. However, it still seems possible to classify a possible type of equation that has exact analytical solutions. In this paper, a method to build this type of equation systematically is presented. An infinite sequence of equations is derived in a kind of recursion form; well-known differential equations like Bessel equations, solutions of which are in analytical form, are taken as the initial equation.

II. BASIC IDEA

We consider the exact solution of

$$\frac{d^2x}{dt^2} + [q_1(t) + \lambda q_2(t)]x = 0, \tag{1}$$

where $q_1(t)$ is continuous in the interval of interest, $q_2(t)$ is a positive and twice continuously differentiable function, and λ is an arbitrary constant. Using the Liouville and Green transformation,[1]

$$s = \phi(t), \quad y = \psi(t)x(t), \tag{2}$$

we change (1) into

$$\frac{d^2y}{ds^2} + \frac{1}{\dot\phi^2}\left(\ddot\phi - \frac{2\dot\phi\dot\psi}{\psi}\right)\frac{dy}{ds} + \frac{1}{\dot\phi^2}\left[q_1 + \lambda q_2 - \frac{\ddot\psi\psi - 2\dot\psi^2}{\psi^2}\right]y = 0, \tag{3}$$

where overdots denote differentiations with respect to t. Choosing ϕ and ψ such that

$$\ddot\phi - 2\dot\phi\dot\psi/\psi = 0 \quad \text{and} \quad q_2 = \dot\phi^2 \tag{4}$$

or

$$\phi = \int [q_2(t)]^{1/2}\,dt, \quad \psi = [q_2(t)]^{1/4}, \tag{5}$$

we reduce (3) to

$$\frac{d^2y}{ds^2} + \left(\lambda + \frac{q_1}{q_2} - \frac{\ddot q_2}{4q_2^2} + \frac{5}{16}\frac{\dot q_2^2}{q_2^3}\right)y = 0. \tag{6}$$

For later convenience, using the transformation $q_2 = \beta^{-2}$, we write Eq. (6) as follows:

$$\frac{d^2y}{ds^2} + \left[\lambda + \left(\frac{1}{2}\beta\ddot\beta - \frac{1}{4}\dot\beta^2 + q_1(t)\beta^2\right)\right]y = 0. \tag{7}$$

If the term parenthesized in Eq. (7) is constant, Eq. (7) has two independent solutions; that is,

$$y_{1,2} = \exp(\pm i\sqrt{\lambda + C}\cdot s) \tag{8}$$

with

$$C = \tfrac{1}{2}\beta\ddot\beta - \tfrac{1}{4}\dot\beta^2 + q_1(t)\beta^2. \tag{9}$$

Here, note that the auxiliary function[2] of the second-order ordinary differential equation of the form

$$\ddot x + q_1(t)x = 0 \tag{10}$$

is well known to satisfy

$$\tfrac{1}{2}\beta\ddot\beta - \tfrac{1}{4}\dot\beta^2 + q_1(t)\beta^2 = 1. \tag{11}$$

It should be noted that there is the following relationship between β in this paper and ρ and h in Ref. 2: $\beta = \rho^2$, $h = 1$. Its solution is described in terms of the independent solutions $x_{1,2}^0$ of Eq. (10) as follows[3,4]:

$$\beta(t) = c_1(x_1^0)^2 + c_2(x_2^0)^2 + 2\sqrt{c_1c_2 - 1/W^2}\,x_1^0x_2^0, \tag{12}$$

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where W is the Wronskian, and c_1 and c_2 are arbitrary constants. Thus, if we take the inverse square of the above auxiliary function as $q_2(t)$, the solution for Eq. (1) can be always written in the form of

$$x_{1,2}(t) = \sqrt{\beta(t)}\exp\left[\pm i\sqrt{\lambda+1}\int\frac{dt}{\beta(t)}\right]. \tag{13}$$

For an analytical expression for solution (13), it is essential that the independent solutions of (10), that is, $x^0_{1,2}$, are in analytical form.

In addition, the above results suggest that there is a class of solvable differential equations uniquely determined from an initial equation of the form

$$\ddot{x}+f_0(t)x=0. \tag{14}$$

We have an infinite sequence of such equations

$$\ddot{x}+\left[f_0(t)+\sum_{i=1}^{N}\frac{\lambda_i}{\beta_i^2}\right]x=0 \quad (N=1,2,3,\ldots,\infty) \tag{15}$$

associated with

$$\frac{1}{2}\beta_N\ddot{\beta}_N-\frac{1}{4}\dot{\beta}_N^2+\left[f_0(t)+\sum_{i=1}^{N-1}\frac{\lambda_i}{\beta_i^2}\right]\beta_N^2=1, \tag{16}$$

and their solutions can be described in the form of recursion equations

$$x^N_{1,2}(t)=\sqrt{\beta_N(t)}\exp\left[\pm i\sqrt{\lambda_N+1}\int\frac{dt}{\beta_N(t)}\right], \tag{17}$$

$$\begin{aligned}\beta_N(t)=\beta_{N-1}\Bigg[&c_1\exp\left(2i\sqrt{\lambda_{N-1}+1}\int\frac{dt}{\beta_{N-1}}\right)\\&+c_2\exp\left(-2i\sqrt{\lambda_{N-1}+1}\int\frac{dt}{\beta_{N-1}}\right)\\&+2\sqrt{c_1c_2+\frac{1}{4(\lambda_{N-1}+1)}}\Bigg].\end{aligned} \tag{18}$$

Here, note that the independent solutions for the initial equation (14) are referred to as the initial solutions throughout the paper.

III. EXAMPLES

As examples, let us consider the case of $f_0(t)=\alpha t^{\nu}$.

A. Case 1: $\nu=0$ and $\alpha=0$

From the initial equation $\ddot{x}=0$, we readily have the auxiliary function $\beta_1(t)=at^2+bt+c$ with $a=(4+b^2)/4c$. This leads to the first part of the infinite sequence,

$$\ddot{x}+[\lambda/(at^2+bt+c)^2]x=0, \tag{19}$$

and its independent solution is described by

$$x_{1,2}(t)=\sqrt{at^2+bt+c}\exp\left(\pm i\sqrt{\lambda+1}\int\frac{dt}{at^2+bt+c}\right). \tag{20}$$

Since the integral of Eq. (20) reduces to

$$\frac{2}{\sqrt{4ac-b^2}}\tan^{-1}\left(\frac{2at+b}{\sqrt{4ac-b^2}}\right) \quad \text{or} \quad \tan^{-1}\left(at+\frac{b}{2}\right),$$

we obtain

$$\begin{aligned}x_{1,2}(t)&=\sqrt{at^2+bt+c}\\&\quad\times\exp[\pm i\sqrt{\lambda+1}\tan^{-1}(at+b/2)].\end{aligned} \tag{21}$$

Equations (21) is in agreement with the result given in the textbook[5] by Magnus and Winkler.

B. Case 2: $\nu=0$ and $\alpha\neq0$

The initial equation is $\ddot{x}+\alpha x=0$. This has the auxiliary function described by

$$\beta_1(t)=\sqrt{C^2+1/\alpha}+C\cos(2\sqrt{\alpha}t+\phi_0), \tag{22}$$

where C and ϕ_0 are arbitrary constants. From (22), we have the first part of the infinite sequence,

$$\ddot{x}+[\alpha+\lambda/(\sqrt{C^2+1/\alpha}+C\cos(2\sqrt{\alpha}t+\phi_0))^2]x=0, \tag{23}$$

and its independent solution is given by

$$\begin{aligned}x_{1,2}(t)&=[\sqrt{C^2+1/\alpha}+C\cos(2\sqrt{\alpha}t+\phi_0)]^{1/2}\\&\quad\times\exp\left[\pm i\sqrt{\lambda+1}\right.\\&\quad\left.\times\int\frac{dt}{\sqrt{C^2+1/\alpha}+C\cos(2\sqrt{\alpha}t+\phi_0)}\right].\end{aligned} \tag{24}$$

Since the integral also reduces to

$$\begin{aligned}&\int\frac{dt}{\sqrt{C^2+1/\alpha}+C\cos(2\sqrt{\alpha}t+\phi_0)}\\&\quad=\frac{1}{2}\sin^{-1}\left(\frac{\sqrt{1/\alpha}\sin(2\sqrt{\alpha}t+\phi_0)}{\sqrt{C^2+1/\alpha}+C\cos(2\sqrt{\alpha}t+\phi_0)}\right),\end{aligned}$$

Eq. (24) becomes

$$\begin{aligned}x_{1,2}(t)&=\left[\sqrt{c^2+1/\alpha}+C\cos(2\sqrt{\alpha}t+\phi_0)\right]^{1/2}\\&\quad\times\exp\left[\pm\frac{i\sqrt{\lambda+1}}{2}\right.\\&\quad\left.\times\sin^{-1}\left(\frac{\sqrt{1/\alpha}\sin(2\sqrt{\alpha}t+\phi_0)}{\sqrt{C^2+1/\alpha}+C\cos(2\sqrt{\alpha}t+\phi_0)}\right)\right].\end{aligned} \tag{25}$$

For the case of $\alpha<0$, the auxiliary function is

$$\beta_1(t)=\sqrt{C^2-1/\alpha}+C\cosh(2\sqrt{-\alpha}t+\phi_0).$$

Therefore, the independent solution is written as follows:

$$\begin{aligned}&x_{1,2}(t)\\&\quad=[\sqrt{C^2-1/\alpha}+C\cosh(2\sqrt{-\alpha}t+\phi_0)]^{1/2}\\&\qquad\times\exp\pm i\sqrt{\lambda+1}\tan^{-1}[(\sqrt{-\alpha}C-\sqrt{-\alpha C^2-1})\\&\qquad\times\tanh(\sqrt{-\alpha}t+\phi_0/2]\},\end{aligned} \tag{26}$$

where the integral formula

$$\begin{aligned}&\int\frac{dt}{\sqrt{C^2-1/\alpha}+C\cosh(2\sqrt{-\alpha}t+\phi_0)}\\&\quad=\tan^{-1}[(\sqrt{-\alpha}C-\sqrt{-\alpha C^2-1})\\&\qquad\times\tanh(\sqrt{-\alpha}t+\phi_0/2)]\end{aligned}$$

is used.

C. Case 3: $\nu = 1$ and $\alpha \neq 0$

The initial equation is $\ddot{x} + \alpha t x = 0$. This auxiliary function[3,4] is described by

$$\beta(t) = \left(\frac{\pi}{3}\right)^2 t\left[aN_\mu^2\left(\frac{2}{3}\sqrt{\alpha}t^{3/2}\right) + bJ_\mu^2\left(\frac{2}{3}\sqrt{\alpha}t^{3/2}\right) + 2\sqrt{ab - \frac{\pi^2}{9}}N_\mu\left(\frac{2}{3}\sqrt{\alpha}t^{3/2}\right)J_\mu\left(\frac{2}{3}\sqrt{\alpha}t^{3/2}\right)\right], \tag{27}$$

where N and J are Bessel and Neumann functions, μ is $\frac{1}{3}$, and a, b are arbitrary constants. Using (27), we have the first part of the infinite sequence of the form

$$\ddot{x} + \left\{\alpha t + \frac{\lambda}{(\pi/3)^4 t^2\left[aN_\mu^2(\theta) + bJ_\mu^2(\theta) + 2\sqrt{ab - \pi^2/9}N_\mu(\theta)J_\mu(\theta)\right]^2}\right\}x = 0, \tag{28}$$

with $\theta = \frac{2}{3}\sqrt{\alpha}t^{3/2}$. Thus the independent solution is written as

$$x_{1,2}(t) = \frac{\pi}{3}\left\{t\left[aN_\mu^2(\theta) + bJ_\mu^2(\theta) + 2\sqrt{ab - \frac{\pi^2}{9}}N_\mu(\theta)J_\mu(\theta)\right]\right\}^{1/2} \times \exp\left\{\pm i\frac{9}{\pi^2}\sqrt{\lambda + 1}\int \frac{dt}{t\left[aN_\mu^2(\theta) + bJ_\mu^2(\theta) + 2\sqrt{ab - \pi^2/9}N_\mu(\theta)J_\mu(\theta)\right]}\right\}. \tag{29}$$

IV. DISCUSSION

As seen in Secs. II and III, a sequence of equations is uniquely determined from the initial equation. In addition to the equations mentioned in Sec. III, we can take into account other equations as possible candidates to replace the initial equation; that is, many of the equations that reduce to Bessel equations, the Mathieu equation, the Whittaker equation, and the Weber equation, because their solutions are in analytical forms.

It is notable that equations built by the present technique have apparent stability characteristics. They depend on both an initial solution (bounded or unbounded) and the value of λ ($\lambda < -1$ or $\lambda \geq -1$): (1) for the case of a bounded initial solution, $\lambda \geq -1$ solutions for equations built from this initial equation are always bounded; (2) for the cases of a bounded initial solution, $\lambda < -1$ or an unbounded initial solution, $\lambda \geq -1$ solutions diverge oscillating; and (3) for the case of an unbounded initial solution, $\lambda < -1$, solutions monotonously diverge.

In accelerator physics, there exist typical applications of the mathematical results for the present examples; they are the linearized Kapchinskij–Vladimirskij (KV) envelope equations[6] in a magnetic focusing channel and a periodic beam–beam focusing system. Since the details of a discussion on those applications are beyond our current scope, they will be presented elsewhere.[7,8]

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Wave equations with the characteristic propagation property

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Within the class of second-order linear self-adjoint wave equations in 1 + 1 dimensions, an explicit construction is given of probably all those with the characteristic propagation property, that is, those whose solutions are without tails.

I. INTRODUCTION

It is the purpose of this paper to explicitly construct a family of self-adjoint second-order hyperbolic partial differential equations in one space dimension with simple mathematical properties. It is likely that all such equations are obtained. The special equations that are sought have solutions with what Kundt and Newman[1] have called the *characteristic propagation property* (CPP). Familiar equations that have this property are the ordinary wave equation in one dimension,

$$\partial_{uv}\Psi = 0;$$

the radial wave equations that result from separating the Minkowski space D'Alembertian in spherical coordinates

$$\left[\partial_{uv} + \frac{1}{u+v}(\partial_u + \partial_v) - \frac{l(l+1)}{(u+v)^2}\right]\Phi_l = 0,$$

l a positive integer;

and wave equations in one dimension involving the "reflectionless" Bargmann potentials,

$$\left[\partial_{uv} + \frac{1}{u+v}(\partial_u + \partial_v) - \frac{l(l+1)}{\cosh^2(u+v)}\right]\chi_l = 0,$$

l a positive integer.

The mathematical simplicity of these equations is reflected in their closed form general solutions. For example,

$$\Psi = a(u) + b(v)$$

for the first one, and

$$\Phi_0 = \frac{a(u) + b(v)}{(u+v)},$$

$$\Phi_1 = \frac{\dot{a}(u) + \dot{b}(v)}{u+v} - \frac{2a(u) + 2b(v)}{(u+v)^2},$$

etc.

for the second set. It will be convenient to speak of such solutions as CP solutions, and of the corresponding wave equations as having the CPP and of being CP equations.

The definition of the CPP is reviewed in Sec. II. In addition we there review the *substitution sequence* (SS) generated by the coefficients of any one-dimensional linear wave equation, self-adjoint or not. The SS was introduced in Ref. 1 because its termination is obviously sufficient, and probably necessary, for the original equation to be a CP equation. The condition that the SS first yields a vanishing term, i.e., terminates, after N steps is a nonlinear partial differential equation of order $2N$. Although a variety of particular solutions of this nonlinear condition are known,[1–4] there has been no suggestion as to the form its general solution might take.

In Sec. III we introduce a set of N new dependent variables in terms of which the termination condition takes the form of a system of N coupled second-order nonlinear evolution equations. The system is complicated; however, for the case $N = 1$, it is the well-known Liouville equation[5] $\sigma_{uv} = e^{\sigma}$. As the general solution of this equation is known, and relatively simple, one is encouraged regarding the general case. Similar systems of nonlinear evolution equations have in fact been studied, and solved, by Leznov[6] and Leznov and Saveliev.[7] Beginning with one of their systems of $2N$ equations and its general solution, we obtain the general solution of our system of N equations for the case where the original wave equation was self-adjoint. If the termination of the SS is, as seems likely, necessary for the CPP, as well as sufficient for it, then all self-adjoint CP equations of second order in the one-dimensional setting have been obtained. In any case, the number and variety of such equations that can be explicitly written down has been greatly enlarged.

II. REVIEW OF CHARACTERISTIC PROPAGATION AND SUBSTITUTION SEQUENCES

Consider the equation

$$\sum_{a,b=1}^{2} g^{ab}(x^c)\Phi_{;ab} + \sum_{a=1}^{2} h^a(x^c)\Phi_{;a} + i(x^c)\Phi = 0, \quad (1)$$

where g^{ab} has signature 0. A combination of a coordinate transformation on x^1, x^2, a conformal transformation on g^{ab}, and a factor transformation on Φ can always be found,[1] which will transform (1) to either of two forms:

$$\{\partial_v k(u,v)\partial_u - j(u,v)\}\Psi(u,v) = 0, \quad (2a)$$

$$\{\partial_u \tilde{k}(u,v)\partial_v - \tilde{j}(u,v)\}\tilde{\Psi}(u,v) = 0, \quad (2b)$$

In this paper we are concerned only with examples of (1) that are self-adjoint, which means that $k(u,v)$ and $\tilde{k}(u,v)$ are constant, so (2a) and (2b) coincide, and we can thus begin our discussion with

$$\{\partial_{vu} - j_1(u,v)\}\Psi_1(u,v) = 0; \quad (3)$$

the subscripts on j_1 and Ψ_1 anticipate future developments.

In order to define what it means for (3) to be a CP equation, we consider its characteristic initial data problem. Suppose u_0, v_0 label two intersecting characteristics and $\Psi_1(u_0,v) = a(v)$, $\Psi_1(u,v_0) = b(u)$. Suppose that if $a(v) \neq 0 \Rightarrow v_1 \leqslant v \leqslant v_2$ and $b(u) \neq 0 \Rightarrow u_1 \leqslant u \leqslant u_2$, then $\Psi_1(u,v) \neq 0 \Rightarrow u_1 \leqslant u \leqslant u_2$ or $v_1 \leqslant v \leqslant v_2$; in this case we say that (3) is a CP equation and its solutions are CP waves. In simple terms, it means that characteristic initial data whose support is initially between two characteristics generates a field whose support remains between them.

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An ingenious approach to finding CP equations was presented in Ref. 1. If we define j_2 and Ψ_2 by $j_2 = j_1[j_1 - \partial_{uv} \ln|j_1|]$, $\Psi_1 = \partial_v(j_1\Psi_2)$ it is a simple matter to confirm that (3) is equivalent to $(\partial_v j_1 \partial_u - j_2)\Psi_2 = 0$. More generally if we inductively define j_n, Ψ_n, $n = 2,3,...,N$, by

$$\frac{j_{n+1}}{j_n} = \frac{j_n}{j_{n-1}} - \partial_{uv} \ln|j_n|, \quad j_n\Psi_n = \partial_v(j_n\Psi_{n+1}), \tag{4}$$

then (3) is in fact equivalent to any one of

$$(\partial_v j_n \partial_n - j_{n+1})\Psi_{n+1} = 0, \quad n = 1,2,...,N, \tag{5}$$

where we assume that none of $j_1,...,j_N$ vanish. If $j_{N+1} \equiv 0$, we cannot continue generating the sequence of j_n's and of equivalent equations, and we say that the *substitution sequence* $j_1, j_2, j_3,...$ *terminates after N steps*. In such a case it follows that $\partial_v j_N \partial_u(\Psi_{N+1}) = 0$, which is solved by $\Psi_{N+1} = a(v)$, where $a(v)$ is an arbitrary function of v. We can now work our way back to Ψ_1 via (5), and obtain

$$\Psi_1(u,v) = \frac{1}{j_1}\partial_v \frac{j_1}{j_2}\partial_v \frac{j_2}{j_3} \cdots \partial_v \frac{j_{N-1}}{j_N}\partial_v[j_N a(v)], \tag{6a}$$

a solution of (3) depending on an arbitrary function. Starting again with (3) but with ∂_{uv} in place of ∂_{vu} we find that

$$\Psi_1(u,v) = \frac{1}{j_1}\partial_u \frac{j_1}{j_2}\partial_u \frac{j_2}{j_3} \cdots \partial_u \frac{j_{N-1}}{j_N}\partial_u[j_N b(u)] \tag{6b}$$

is also a solution of (3), depending on an arbitrary function of u. The sum of (6a) and (6b) is the general solution of (3). What is more, it is obvious from the form of the general solution that (3) is a CP equation.

Thus every equation that generates a terminating SS is a CP equation. If the sequence does *not* terminate we know of no proof that the equation is *not* a CP equation, but Kundt and Newman plausibly conjecture this to be so. If so, then to find all $j_1(u,v)$'s that generate $j_{N+1}(u,v) = 0$ for some N is to find all self-adjoint CP equations.

Unfortunately, if we concatenate the equations defining $j_1, j_2,..., j_{N+1}$ and set $j_{N+1} = 0$, we obtain a nonlinear differential equation that is of order $2N$ *and* exceedingly complicated. It is this equation which we will rewrite and solve in the next section.

III. SOLVING THE TERMINATION CONDITION

Given a substitution sequence $j_1, j_2,..., j_N$ such that j_{N+1} is the first term that vanishes, let us introduce a new sequence of functions $\sigma_1, \sigma_2,..., \sigma_N$, where $j_1 = e^{\sigma_1}$ while

$$j_n = j_{n-1}e^{\sigma_n}, \quad n = 2,...,N. \tag{7}$$

As we are considering only real-valued functions of real coordinates, this would appear to preclude sequences containing j_n's that are negative, however, none of our analysis would be affected by complex constants added to the σ_n's, so no such restriction is operating. It is a trivial matter to confirm that, given (7),

$$j_2 = 0 \Leftrightarrow \partial_{uv}\sigma_1 = e^{\sigma_1}. \tag{8}$$

Thus termination after one step is equivalent to the classical Liouville equation whose general solution is known, and is usually written in the form

$$e^{\sigma_1} = 2\{U'(u)V'(v)/[U(u) + V(v)]^2\}, \tag{9}$$

where U and V are two arbitrary differentiable functions. To the best of our knowledge it has not been noted earlier that this equation, which occurs in a variety of mathematical and physical contexts, has the significance given to it by (8) as well. It is not difficult to generalize (8) and obtain

$$j_{N+1} = 0 \Leftrightarrow \partial_{uv}\begin{bmatrix}\sigma_1\\ \vdots \\ \sigma_N\end{bmatrix} = K_N\begin{bmatrix}e^{\sigma_1}\\ \vdots \\ e^{\sigma_N}\end{bmatrix}, \tag{10}$$

where the $N \times N$ matrix K_N is given by

$$K_N = \begin{bmatrix} 1 & -1 & 0 & \cdots & & & \\ -1 & 2 & -1 & 0 & \cdots & & \\ 0 & -1 & 2 & -1 & 0 & \cdots & \\ & & & \ddots & & & \\ & \cdots & 0 & -1 & 2 & -1 & 0 \\ & & \cdots & 0 & -1 & 2 & -1 \\ & & & \cdots & 0 & -1 & 2 \end{bmatrix}. \tag{11}$$

On the one hand it is gratifying that the condition for termination after N steps can be written in such a relatively simple form; in particular the matrix K_N is symmetric and tridiagonal. On the other hand, even with the knowledge of a variety of particular solutions of (10), the generalization of (9) to the general solution of (10) is elusive.

From considerations quite independent of any mentioned above, Leznov[6] and Leznov and Saveliev[7] have been led to consider the sytem (10) with K_N replaced by matrices of any one of four distinct types, none of them identical to (11). We shall begin with one of their types, write down its general solution, and by a simple argument obtain from it the general solution of (10).

Consider the system

$$\partial_{uv}\begin{bmatrix}\tau_1\\ \vdots \\ \tau_M\end{bmatrix} = \begin{bmatrix}e^{(A_M\tau)_1}\\ \vdots \\ e^{(A_M\tau)_M}\end{bmatrix}, \tag{12}$$

where the $M \times M$ matrix A_M is given by

$$A_M = \begin{bmatrix} 2 & -1 & 0 & \cdots & & & \\ -1 & 2 & -1 & 0 & \cdots & & \\ 0 & -1 & 2 & -1 & 0 & \cdots & \\ & & & \ddots & & & \\ & \cdots & 0 & -1 & 2 & -1 & 0 \\ & & \cdots & 0 & -1 & 2 & -1 \\ & & & \cdots & 0 & -1 & 2 \end{bmatrix}. \tag{13}$$

Note that not only do (10) and (12) differ in form (it is in fact a superficial difference), but that (11) and (13) differ in one entry (this turns out to be a more significant matter).

For the ingenious argument by which Leznov and Saveliev find the general solution of (12) and (13) the reader is referred to their papers.[6,7] It is sufficient for our purposes to simply restate the result. Consider first the case $M = 1$, that is, the equation

$$\partial_{uv}\tau_1 = e^{2\tau_1}. \tag{14}$$

It is easy to confirm that (14) is solved by

$$e^{\tau_1} = [f'(u)g'(v)]^{1/2}/[f(u)+g(v)], \tag{15}$$

where f and g are arbitrary differentiable functions [(14) and (15) are, of course, simply related to (8) and (9)]. Now let us introduce a new dependent variable $X_1(u,v)$ in place of τ_1, and two new functions φ_1 and Ψ_1 in place of f and g, by

$$X_1 = e^{-\tau_1}, \quad \Psi_1(u) = f'(u), \quad \Psi_1(v) = -[1/g(v)]'. \tag{16}$$

In terms of these new functions (15) becomes

$$e^{-\tau_1} = X_1 = \frac{[\int^u \varphi_1]\,[\int^v \Psi_1] - 1}{[\varphi_1(u)\Psi_1(v)]^{1/2}}. \tag{17}$$

Although (17) is not intrinsically simpler than (15), it turns out that it generalizes more easily to the solution of (12) for $N>1$. Following Refs. 6 and 7 we introduce the operator Δ_m by

$$\Delta_m X(u,v) = \begin{vmatrix} X & X_u & \cdots & X_{\underbrace{u\cdots u}^{m-1}} \\ X_v & X_{vu} & \cdots & X_{\underbrace{u\cdots uv}^{m-1}} \\ \vdots & & \ddots & \vdots \\ X_{\underbrace{v\cdots v}^{m-1}} & X_{\underbrace{v\cdots vu}^{m-1}} & \cdots & X_{\underbrace{v\cdots v}^{m-1}\,\underbrace{u\cdots u}^{m-1}} \end{vmatrix}. \tag{18}$$

It can be confirmed, with patience, that for $M=2$, (12) is solved by

$$e^{-\tau_1} = X_2, \quad e^{-\tau_2} = -\Delta_2 X_2, \tag{19}$$

where

$$X_2(u,v) = \frac{[\int^u \varphi_1 \int \varphi_2]\,[\int^v \Psi_1 \int \Psi_2] - [\int^u \varphi_1]\,[\int^v \Psi_1] + 1}{[\varphi_1^2(u)\varphi_2(u)\Psi_1^2(v)\Psi_2(v)]^{1/3}}. \tag{20}$$

It is shown in Refs. 6 and 7 that, for arbitrary M, (12) is solved by

$$e^{-\tau_m} = (-1)^{m(m-1)/2}\Delta_m X_M(u,v), \quad m = 1,2,\ldots,M, \tag{21}$$

where

$$e^{-\tau_1} = X_M = \frac{[\int^u \varphi_1 \cdots \int \varphi_M]\,[\int^v \Psi_1 \cdots \int \Psi_M] - \cdots + (-1)^{M-1}[\int^u \varphi_1]\,[\int^v \Psi_1] + (-1)^M}{[\varphi_1^M(u)\varphi_2^{M-1}(u)\cdots\varphi_M(u)\Psi_1^M(v)\Psi_2^{M-1}(v)\cdots\Psi_M(v)]^{1/(M+1)}}. \tag{22}$$

It remains to use (21) and (22) to obtain the solution of (10). The crucial step rests, again, on a result in Ref. 6. There it is shown that

$$\left.\begin{array}{ll} \varphi_1 = \varphi_M, & \Psi_1 = \Psi_M \\ \varphi_2 = \varphi_{M-1}, & \varphi_2 = \varphi_{M-1} \\ \vdots & \vdots \end{array}\right\} \Rightarrow \left\{\begin{array}{l} \tau_1 = \tau_M, \\ \tau_2 = \tau_{M-1}, \\ \vdots \end{array}\right. \tag{23}$$

If we take (13) with $M = 2Q$, and assume the hypothesis of (23), the conclusion of (23) shows us that the set of the first Q equations of (12) is identical to the set of the last Q, and this set is a new set. As a result we see that

$$\partial_{uv}\begin{bmatrix} \tau_1 \\ \vdots \\ \tau_Q \end{bmatrix} = \begin{bmatrix} e^{(E_Q\tau)_1} \\ \vdots \\ e^{(E_Q\tau)_Q} \end{bmatrix}, \tag{24}$$

where the $Q\times Q$ matrix E_Q is

$$E_Q = \begin{bmatrix} 2 & -1 & 0 & \cdots & & & \\ -1 & 2 & -1 & 0 & \cdots & & \\ 0 & -1 & 2 & -1 & 0 & \cdots & \\ & & & \ddots & & & \\ & \cdots & 0 & -1 & 2 & -1 & 0 \\ & & \cdots & 0 & -1 & 2 & -1 \\ & & & \cdots & 0 & -1 & 1 \end{bmatrix}, \tag{25}$$

is solved by

$$e^{-\tau_q} = (-1)^{q(q-1)/2}\Delta_q X_Q(u,v), \quad q = 1,\ldots,Q, \tag{26}$$

where

$$e^{-\tau_1} = X_Q = \frac{\Sigma_{j=0}^{2Q}(-1)^j I^j(u) I^j(v)}{\varphi_1(u)\cdots\varphi_Q(u)\Psi_1(v)\cdots\Psi_Q(v)}, \tag{27}$$

with the iterated integral I^j given in terms of j arbitrary functions by $I^0 = 1$ and

$$I^j(u) = \int^u \overbrace{\varphi_1 \int \varphi_2 \cdots \int \varphi_{Q-1} \int \varphi_Q \int \varphi_Q \int \varphi_{Q-1} \cdots \int \varphi_2 \int \varphi_1}^{j}$$
$$I^j(v) = \int^v \underbrace{\Psi_1 \int \Psi_2 \cdots \int \Psi_{Q-1} \int \Psi_Q \int \Psi_Q \int \Psi_{Q-1} \cdots \int \Psi_2 \int \Psi_1}_{j}$$
$$j = 1,2,\ldots,2Q. \tag{28}$$

In (28) the bracket labeled j indicates that I^j is the first j iterated integrals of the full expression; the remaining $2Q-j$ integrals are not present. The next step in our progression from (12) and (13) to (10) and (11) is to set $Q = N$ and to define a new set of dependent variables $\sigma_1',\ldots,\sigma_N'$ by

$$\sigma_1' = \tau_N, \sigma_2' = \tau_{N-1},\ldots,\sigma_N' = \tau_1. \tag{29}$$

The system (24) now becomes

$$\partial_{uv}\begin{bmatrix} \sigma_1' \\ \vdots \\ \sigma_N' \end{bmatrix} = \begin{bmatrix} e^{(K_N\sigma')_1} \\ \vdots \\ e^{(K_N\sigma')_N} \end{bmatrix}, \tag{30}$$

where the $N\times N$ matrix K_N is

$$K_N = \begin{bmatrix} 1 & -1 & 0 & \cdots & & & \\ -1 & 2 & -1 & 0 & \cdots & & \\ 0 & -1 & 2 & -1 & 0 & \cdots & \\ & & \ddots & & & & \\ & \cdots & 0 & -1 & 2 & -1 & 0 \\ & & \cdots & 0 & -1 & 2 & -1 \\ & & & \cdots & 0 & -1 & 2 \end{bmatrix}. \tag{31}$$

The last step is to shift the matrix K_N to its desired position, and this is obviously accomplished by defining

$$\underline{\sigma} = K_N \underline{\sigma}', \text{ i.e., } \begin{cases} \sigma_1 = \sigma_1' - \sigma_2', \\ \sigma_2 = -\sigma_1' + 2\sigma_2' - \sigma_3', \\ \quad \vdots \\ \sigma_{N-1} = -\sigma_{N-2}' + 2\sigma_N' - \sigma_N', \\ \sigma_N = -\sigma_{N-1}' + 2\sigma_N'. \end{cases} \tag{32}$$

The linear combinations on the right-hand side of (32) become products of integer powers when the exponentials of the σ's and σ''s are considered, and it is easy to confirm that, given $I^j(u)$, $I^j(v)$ as in (28), the result is

$$\begin{aligned} j_1 &= (-1)^{N-1}\Delta_{N-1}X_N/\Delta_N X_N, \\ j_2 &= (-1)^{N-2}\Delta_{N-2}X_N/\Delta_{N-1}X_N, \\ j_n &= (-1)^{N-n}\Delta_{N-n}(X_n)/\Delta_{N-n+1}(X_N), \\ j_{N-1} &= -X_N/\Delta_2 X_N, \\ j_N &= +1/X_N, \\ j_{N+1} &= 0, \end{aligned} \tag{33}$$

where

$$X_N = \frac{\Sigma_{j=0}^{2N}(-1)^j I^j(u) I^j(v)}{\varphi_1(u)\cdots\varphi_N(u)\Psi_1(v)\cdots\Psi_N(v)}. \tag{34}$$

Since there are $2N$ arbitrary functions in X_N and j_{N+1} is the first vanishing j_n, (33), and (34) give the general substitution sequence that terminates after N steps, within the class of wave equations that we are considering.

IV. CONCLUSION

With any reasonable definition of "closed form" the wave equations given as examples of CP equations in the Introduction can be said to have general solutions expressible in closed form. From the formulas (6a), and (6b) it is clear that the family of CP equations has this property and may be regarded as a natural generalization of $\partial_{uv}\Psi = 0$ in this sense. This, combined with the fact that these equations can be themselves written down, by means of (33) and (34), in terms of coefficients with an explicit representation, is why we earlier referred to the CP equations as being mathematically simple.

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Linearization of the Hamilton–Jacobi equation

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Through a canonoid transformation the integration for the Hamilton–Jacobi equations is transformed into a two step procedure: the first being a linear problem and the second a quasilinear one. Examples are given.

I. INTRODUCTION

Given the Lagrangian

$$L(q,\dot{q},t) = \sum a_{ij}(q,t)\dot{q}_i\,\dot{q}_j - V(q,t) \quad (i,j = 1,...,N)\,,$$

we have the Hamiltonian

$$H(q,p,t) = \sum b_{ij}(q,t)\,p_i\,p_j + V(q,t) \tag{1}$$

(where $\Sigma b_{ij}\,a_{ik} = \delta_{jk}$).

The corresponding Hamilton–Jacobi equation is

$$f \equiv \sum b_{ij}\frac{\partial S}{\partial q_i}\frac{\partial S}{\partial q_j} + V + \frac{\partial S}{\partial t} = 0\,. \tag{2}$$

Solutions of the Hamilton–Jacobi equations have extensive use: as a fundamental concept in classical mechanics,[1] as a practical tool for solving differential equations,[2] as a basis for quantum mechanics,[3] as a zeroth-order approximation in the WKB method,[4] etc.

Unfortunately, Eq. (2) is a nonlinear partial differential equation—and to solve it is, in general, an almost insurmountable task. This note presents a way of overcoming the problem: a technique for linearizing this equation. Through a canonoid transformation, Eq. (2) is transformed into a linear one and the determination of the adequate canonoid transformation is achieved by solving a quasilinear system.

As an additional advantage, our method leads to the general solution of the Hamilton–Jacobi equation—certainly more important than the usual complete solution.[5]

II. THE LINEARIZATION METHOD

The Hamiltonian—Eq. (1)—is transformed into

$$\overline{H} = \sum A_i\,P_i - \sum a_{ij}\,A_i\,A_j + V, \tag{3}$$

by any member of the family of transformations

$$Q_i = q_i\,,$$

$$\sum A_i\,P_i = \sum b_{ij}\,p_i\,p_j + \sum a_{ij}\,A_i\,A_j\,. \tag{4}$$

It is easy to prove that canonical equations for $\overline{H}$ will describe the same mechanical system provided that the functions A_i obey the set of quasilinear partial differential equations

$$2A_k\frac{\partial}{\partial q_k}\left(\sum a_{li}\,A_l\right) + 2\frac{\partial}{\partial t}\left(\sum a_{li}\,A_l\right) = \sum A_l\,A_m\frac{\partial a_{lm}}{\partial q_i} - \frac{\partial V}{\partial q_i} \quad (i = 1,...,N)\,. \tag{5}$$

(The above equations are derived from the Euler–Lagrange equations in which we use $\dot{q}_i = A_i$.)

Then the Hamilton–Jacobi equation corresponding to $\overline{H}$ is

$$g \equiv \sum A_i\frac{\partial \overline{S}}{\partial q_i} - \sum a_{ij}\,A_i\,A_j + V + \frac{\partial \overline{S}}{\partial t} = 0\,. \tag{6}$$

Since $[f,g] = 0$, it may be assured[6] that Eq. (2) and Eq. (6) will present a common solution—and its determination is much easier if we seek for solutions of Eq. (6), due to its linear character.

III. EXAMPLES

Suppose we have a system described by the Lagrangian

$$L = a\dot{q}_1^2 + a\dot{q}_2^2 - 2q_1 - 2q_2\,,$$

then the corresponding Hamiltonian is

$$H = (p_1^2 + p_2^2)/4a + 2q_1 + 2q_2\,.$$

Its Hamilton–Jacobi equation is given by

$$\frac{1}{4a}\left(\frac{\partial S}{\partial q_1}\right)^2 + \frac{1}{4a}\left(\frac{\partial S}{\partial q_2}\right)^2 + 2q_1 + 2q_2 + \frac{\partial S}{\partial t} = 0\,. \tag{7}$$

The transformation

$$Q_i = q_i\,,$$

$$\sum A_i\,P_i = \frac{\Sigma p_i^2}{4a} + a\sum A_i^2 \quad (i = 1,2)\,, \tag{8}$$

will be canonoid whenever

$$aA_1\frac{\partial A_i}{\partial q_1} + aA_2\frac{\partial A_i}{\partial q_2} = -1\,, \quad (i = 1,2)\,.$$

This system of equations have the solutions given by

$$aA_i^2 + 2q_i = F_i(A_1 - A_2) \quad (i = 1,2)\,. \tag{9}$$

The new Hamiltonian–Jacobi equation becomes

$$\sum A_i\frac{\partial \overline{W}}{\partial q_i} - aA_1^2 - aA_2^2 + 2q_1 + 2q_2 = \overline{\gamma} \tag{10}$$

[where the separation of variables $\overline{S}(q,t) = \overline{W}(q) - \overline{\gamma}\,t$ was performed, and $\overline{\gamma}$ is the separation constant].

Now, we must perform the integration of the auxiliary system:

$$\frac{dq_1}{A_1} = \frac{dq_2}{A_2} = \frac{d\overline{W}}{\overline{\gamma} + aA_1^2 + aA_2^2 - 2q_1 - 2q_2}\,.$$

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This has the general solution

$$\bar{W} = -\alpha A_2[\bar{\gamma} + \alpha A_2^2/3 - 2q_1 - 2q_2 + \alpha A_1^2 - 2\alpha A_1 A_2] + G(A_1 - A_2), \quad (11)$$

where A_1 and A_2 are given by Eq. (9), and G is an arbitrary function of the variable $(A_1 - A_2)$.

For sake of comparison, let us consider the Hamilton–Jacobi equation, corresponding to the original Hamiltonian—Eq. (7)—

$$\frac{1}{4\alpha}\left(\frac{\partial W}{\partial q_1}\right)^2 + \frac{1}{4\alpha}\left(\frac{\partial W}{\partial q_2}\right)^2 + 2q_1 + 2q_2 = \gamma,$$

where $S = W(q) - \gamma t$.

By Eq. (4), where P_i is considered as $\partial \bar{S}/\partial Q_i = \partial \bar{S}/\partial q_i$ and $p_i = \partial S/\partial q_i$, we can conclude that

$$\gamma = \bar{\gamma}.$$

This Hamilton–Jacobi equation has a solution obtained via separation of variables given by

$$W = -\tfrac{2}{3}\sqrt{\alpha(\gamma - 2q_1 - C)^3} - \tfrac{2}{3}\sqrt{\alpha(C - 2q_2)^3} + C',$$

where C is the separation constant and C' is a constant.

This solution also must be a solution of the linear Hamilton–Jacobi equation—Eq. (10)—i.e.,

$$2A_1\sqrt{\alpha(\gamma - 2q_1 - C)} + 2A_2\sqrt{\alpha(C - 2q_2)} = \gamma - 2q_1 - 2q_2 + \alpha A_1^2 + \alpha A_2^2,$$

which implies in the choice

$$A_1 = \sqrt{(\gamma - 2q_1 - C)/\alpha} \quad \text{and} \quad A_2 = \sqrt{(C - 2q_2)/\alpha},$$

or by Eq. (9) in

$$F_1 = \gamma - C \quad \text{and} \quad F_2 = C.$$

It is easy to prove that $\bar{W}$, given by Eq. (11), reduces to W with the above values for A_1 and A_2 and the arbitrary function $G = \frac{2}{3}\alpha^2(A_2 - A_1)^3 + C'$.

As another example consider the Lagrangian

$$L = \dot{q}_1\dot{q}_2 - q_1 q_2,$$

and the corresponding linear Hamilton–Jacobi equation

$$A_1\frac{\partial \bar{W}}{\partial q_1} + A_2\frac{\partial \bar{W}}{\partial q_2} - A_1 A_2 + q_1 q_2 = \bar{\gamma}$$

(where $\bar{S} = \bar{W} - \bar{\gamma}t$).

Then its general solution is

$$\bar{W} = \gamma \arcsin\frac{q_1}{\sqrt{A_1^2 + q_1^2}} + \frac{q_1[A_1^2 A_2 + q_1^2 A_2]}{q_1^2 + A_2^2} + G(A_1 A_2 + q_1 q_2),$$

with the relations

$$A_i^2 + q_i^2 = F_i(A_1 A_2 + q_1 q_2) \quad (i = 1,2).$$

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Characteristic functional structure of infinitesimal symmetry mappings of classical dynamical systems. III. Systems with cyclic variables

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This paper is a continuation of previous papers I and II with similar titles [J. Math. Phys. **26**, 3080, 3100 (1985)]. In those papers a theory was developed that described the characteristic functional structures of infinitesimal symmetry mappings of systems of first- or second-order dynamical equations. Now an investigation is made of how cyclic variables of the dynamical equations affect the symmetry equations and thereby propagate through the theory to influence the form of the characteristic functional structure of the symmetries. These special symmetries, which have a particularly simple form, are characterized by infinitesimal point mappings in which only cyclic coordinates are varied, with the variation essentially determined by *constants of motion* of the dynamical system. For Lagrangian systems with cyclic coordinates these special symmetry mappings include the well-known Noether symmetries characterized by *constant* variation of the cyclic coordinates.

I. INTRODUCTION

In the preceding papers of this series[1,2] several theorems were developed that described the *characteristic functional structures* of infinitesimal symmetry mappings of systems of first- or second-order ordinary differential equations. A principal feature of the characteristic structures of such mappings is determined by the fundamental solution functions of auxiliary systems of ordinary linear differential equations. These linear equations are obtained by a procedure that uses certain basic properties of both the original (dynamical) differential equations and their associated system of partial differential symmetry equations.

We now investigate how cyclic (missing) variables in the dynamical equations affect the form of the above-mentioned associated system of ordinary *linear* equations and thence the form of their fundamental solution functions and ultimately the functional structure of the symmetry mappings. It will be shown that these resulting special symmetries have a particularly simple form characterized by infinitesimal point mappings in which only cyclic coordinates are varied, with their variations essentially determined by *constants of motion* of the dynamical system. For Lagrangian systems with cyclic coordinates these special symmetry mappings are more general than the well-known classical Noether symmetries characterized by *constant* variations of the cyclic coordinates.

By use of the theory of characteristic functional structure, symmetry mappings are obtained for the following situations: (1) second-order dynamical equations with cyclic coordinate or pairs of cyclic variables, (2) first-order dynamical systems with cyclic coordinates, including a special application for autonomous systems, and (3) first-order systems obtained from the reduction of second-order systems with pairs of cyclic variables.

II. SPECIAL SYMMETRY MAPPINGS OF SYSTEMS OF SECOND-ORDER DYNAMICAL EQUATIONS WITH CYCLIC VARIABLES

As a prerequisite to examining how cyclic variables of a second-order dynamical system lead to special symmetry mappings we summarize elements of characteristic functional structure theory essential to this analysis. For a detailed discussion see Ref. 1.

Consider then a system of second-order dynamical equations of the form[3]

$$\ddot{x}^i = F^i(\dot{x}^1,...,\dot{x}^n;x^1,...,x^n;t) \equiv F^i(\dot{x},x,t), \quad i = 1,...,n, \tag{2.1}$$

with solutions

$$x^i = \phi^i(c^1,...,c^{2n},t) \equiv \phi^i(c,t), \quad c^A = \text{const}, \quad A = 1,...,2n, \tag{2.2}$$

so that upon differentiation

$$\dot{x}^i = \frac{\partial \phi^i}{\partial t}. \tag{2.3}$$

Inversion of (2.2) and (2.3) gives $2n$ functionally independent constants of motion[4]

$$C^A(\dot{x},x,t) \overset{t}{=} c^A. \tag{2.4}$$

An infinitesimal *velocity-dependent* mapping of the form

$$\bar{x}^i = x^i + \delta x^i, \quad \delta x^i \equiv \xi^i(\dot{x},x,t)\delta a, \tag{2.5}$$

$$\bar{t} = t + \delta t, \quad \delta t \equiv \xi^0(\dot{x},x,t)\delta a, \tag{2.6}$$

which maps the set of all solution curves of (2.1) into itself, is defined to be a *velocity-dependent* symmetry mapping of

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the dynamical system (2.1). Such symmetry mappings are expressible in the form

$$\bar{x}^i = x^i + [Z^i(\dot{x},x,t) + \dot{x}^i\xi^0(\dot{x},x,t)]\delta a, \tag{2.7}$$

$$\bar{t} = t + \xi^0(\dot{x},x,t)\delta a, \quad \xi^0 \text{ arbitrary}, \tag{2.8}$$

where $Z^i(\dot{x},x,t)$ is a solution of the system of *partial* differential equations obtained by the formal expansion of the equations[5,6]

$$\ddot{Z}^i + J^i{}_j(\dot{x},x,t)\dot{Z}^j + K^i{}_j(\dot{x},x,t)Z^j \overset{0}{=} 0, \tag{2.9}$$

where [refer to (2.1)]

$$J^i{}_j(\dot{x},x,t) \equiv -\frac{\partial F^i(\dot{x},x,t)}{\partial \dot{x}^j}, \tag{2.10}$$

$$K^i{}_j(\dot{x},x,t) \equiv -\frac{\partial F^i(\dot{x},x,t)}{\partial x^j}. \tag{2.11}$$

Every solution $Z^i(\dot{x},x,t)$ of the partial differential equations obtained from the expansion of (2.9) is expressible in a form with characteristic functional structure[5]

$$Z^i(\dot{x},x,t) = B^A(\dot{x},x,t)g^i_A[C^1(\dot{x},x,t),...,C^\sigma(\dot{x},x,t),t],$$
$$0 \leqslant \sigma \leqslant 2n, \quad A = 1,...,2n, \tag{2.12}$$

where the functions $B^A(\dot{x},x,t)$ are arbitrary constants of motion of the dynamical system (2.1) and the functions $C^A(\dot{x},x,t)$ are the specific constants of motion (2.4). The functions $g^i_A(C,t)$, which appear in (2.12), are obtained by replacing the constants c^A, which appear in functions $g^i_A(c,t)$, with the respective constants of motion C^A by means of (2.4); the functions $g^i_A(c,t)$ are the fundamental solution functions, which occur in the solutions

$$z^i(c,t) = b^A g^i_A(c,t), \quad b^A = \text{const}, \tag{2.13}$$

of an associated system of linear equations

$$\ddot{z}^i + j^i{}_a(c,t)\dot{z}^a + k^i{}_a(c,t)z^a \overset{t}{=} 0, \tag{2.14}$$

obtained from (2.9) and (2.10), where[4]

$$z^i(c,t) \overset{t}{=} Z^i(\dot{x},x,t), \tag{2.15}$$

$$j^i{}_a(c,t) \overset{t}{=} J^i{}_a(\dot{x},x,t), \tag{2.16}$$

$$k^i{}_a(c,t) \overset{t}{=} K^i{}_a(\dot{x},x,t). \tag{2.17}$$

It follows that each fundamental solution function $g^i_A(c,t)$ will satisfy

$$\ddot{g}^i_A + j^i{}_a(c,t)\dot{g}^a_A + k^i{}_a(c,t)g^a_A \overset{t}{=} 0. \tag{2.18}$$

We now use characteristic functional structure theory (outlined above) to show that dynamical systems (2.1) with cyclic coordinates or pairs of cyclic variables admit certain symmetry mappings with special forms.

The dynamical system (2.1) is said to be cyclic in a coordinate x^r if

$$\frac{\partial F^i(\dot{x},x,t)}{\partial x^r} = 0. \tag{2.19}$$

It is to be noted that for a coordinate x^r to be cyclic it must be missing from *every* function $F^i(\dot{x},x,t)$, $i = 1,...,n$. Similarly a dynamical system (2.1) is said to be cyclic in the pair of variables $(x^s, \dot{x}^s)$ if

$$\frac{\partial F^i(\dot{x},x,t)}{\partial x^s} = 0, \quad \frac{\partial F^i(\dot{x},x,t)}{\partial \dot{x}^s} = 0, \quad i = 1,...,n. \tag{2.20}$$

It is now apparent how missing variables in the functions $F^i(\dot{x},x,t)$ of the dynamical equations (2.1) affect the functional structure of $J^i{}_j$ and $K^i{}_j$ [see (2.10) and (2.11)] in the symmetry condition (2.9), and thence [see (2.16) and (2.17)] the structure of the associated system of linear equations (2.14) [and (2.18)].

Consider first the case of the special symmetry solution of (2.9), which is a consequence of a pair of cyclic variables $(x^s, \dot{x}^s)$ in the dynamical system (2.1). In this case we observe that the following g^i_A will be the solution of (2.18):

$$g^i_A = \mu^i_A t + \nu^i_A, \quad \mu^s_A, \nu^s_A = \text{arbitrary constants},$$
$$\mu^i_A = 0, \quad \nu^i_A = 0, \quad i \neq s. \tag{2.21}$$

For the case in which the dynamical system (2.1) is cyclic in a coordinate x^r [but $(x^r, \dot{x}^r)$ not a cyclic pair] the following g^i_A will satisfy (2.18):

$$g^i_A = \nu^i_A, \quad \nu^r_A = \text{arbitrary constants},$$
$$\nu^i_A = 0, \quad i \neq r. \tag{2.22}$$

For both cases considered above the fundamental solution functions g^i_A [(2.21) and (2.22)] are independent of the constants c^A that appear in (2.2) and (2.4). Hence for these two cases of dynamical equations with cyclic variables the above-described g^i_A may be used without modification in (2.12) to obtain symmetry functions $Z^i(\dot{x},x,t)$. This leads to the following theorem.

Theorem 2.1: A dynamical system

$$\ddot{x} = F^i(\dot{x},x,t), \quad i = 1,...,n, \tag{2.1'}$$

will admit an infinitesimal velocity-dependent symmetry mapping

$$\bar{x}^i = x^i + [Z^i(\dot{x},x,t) + \dot{x}^i\xi^0(\dot{x},x,t)]\delta a, \tag{2.7'}$$

$$\bar{t} = t + \xi^0(\dot{x},x,t)\delta a, \quad \xi^0 \text{ arbitrary}, \tag{2.8'}$$

of a special form if the dynamical system is cyclic in (a) a pair of variables $(x^s, \dot{x}^s)$, in that $\partial F^i/\partial x^s = 0$ and $\partial F^i/\partial \dot{x}^s = 0$, $i = 1,...,n$, in which case the Z^i in (2.7') will have the special form

$$Z^s = M^{(s)}(\dot{x},x,t)t + N^{(s)}(\dot{x},x,t), \tag{2.23}$$

$$Z^i = 0, \quad i \neq s; \tag{2.24}$$

and (b) a coordinate x^r, in that $\partial F^i/\partial x^r = 0$, $i = 1,...,n$ [$(x^r, \dot{x}^r)$ not a cyclic pair], in which case the Z^i in (2.7') will have the special form

$$Z^r = N^{(r)}(\dot{x},x,t), \tag{2.25}$$

$$Z^i = 0, \quad i \neq r, \tag{2.26}$$

where $M^{(s)}$, $N^{(s)}$, and $N^{(r)}$ are arbitrary constants of motion of (2.1): ■

Remark 2.1: We have used *characteristic functional structure theory* to examine how missing variables in the dynamical equations affect various elements of the theory and thereby determine symmetry mappings with a special form.

If one were not interested in the details of how cyclic variables affect the characteristic functional structure of the symmetry mappings the simplicity of this particular problem clearly allows one to deduce the form of these special symmetries directly from the symmetry equation (2.9) by taking into account the effect of the missing variables on the functions J_j^i (2.10) and K_j^i (2.11). ■

Remark 2.2: If in Theorem 2.1 we choose $\xi^0(\dot{x},x,t)=0$, and choose the *constants of motion* $M^{(s)}$, $N^{(s)}$, and $N^{(r)}$ to be arbitrary *constants*, then the mappings described in Theorem 2.1 reduce to classical velocity-independent mappings. For the case in which Theorem 2.1 (b) is applicable to a Lagrangian system the above choices for ξ^0 and $N^{(r)}$ lead to the well-known Noether mappings associated with cyclic coordinates. ■

Remark 2.3: If a dynamical system (2.1) is cyclic in *all* $\dot{x}$'s, then the functions $j_a^i(c,t)=0$ [see (2.10) and (2.16)] and the associated system of linear equations (2.14) reduces to that of a time-dependent harmonic oscillator. ■

III. SPECIAL SYMMETRY MAPPINGS OF SYSTEMS OF FIRST-ORDER DYNAMICAL EQUATIONS WITH CYCLIC COORDINATES

For dynamical systems of first order we state Theorem 3.1 without proof, since the proof is similar to that of Theorem 2.1 (b).

Theorem 3.1: A dynamical system

$$\dot{y}^I=\lambda^I(y^1,...,y^N),\quad I=1,...,N, \tag{3.1}$$

will admit an infinitesimal velocity-independent symmetry mapping

$$\bar{y}^I=y^I+[U^I(y,t)+\lambda^I(y,t)\eta^0(y,t)]\delta a, \tag{3.2}$$

$$\bar{t}=t+\eta^0(y,t)\delta a,\quad \eta^0(y,t)\ \text{arbitrary}, \tag{3.3}$$

iff U^I satisfies the symmetry condition[5,7]

$$\dot{U}^I-\frac{\partial\lambda^I}{\partial y^J}U^J\overset{0}{=}0. \tag{3.4}$$

Corresponding to each cyclic coordinate y^R of (3.1) (in that $\partial\lambda^I/\partial y^R=0$) the system (3.1) will admit a transformation (3.2) and (3.3) in which

$$U^R=N^{(R)}(y,t), \tag{3.5}$$

$$U^I=0,\quad I\neq R, \tag{3.6}$$

where $N^{(R)}$ is an arbitrary constant of motion. ■

First-order dynamical systems expressible in the form

$$\dot{y}^I-\lambda^I(y)=0,\quad I=1,...,N, \tag{3.7}$$

are said to be autonomous since the functions λ^I are independent of t.

It is known [8–10] there exist coordinate transformations

$$y^{*A}=f^A(y),\quad \det\left(\frac{\partial y^{*A}}{\partial y^B}\right)\neq 0, \tag{3.8}$$

such that in the y^* coordinates the contravariant vector components $\lambda^{*I}(y^*)$ reduce to the form

$$\lambda^{*I}(y^*)=\delta^I_N. \tag{3.9}$$

In this y^* ("straightened-out") system, the dynamical equations (3.7) reduce to

$$\dot{y}^{*I}-\delta^I_N=0, \tag{3.10}$$

which are cyclic in all of the coordinates y^{*I}. Hence in this coordinate system Theorem 3.1 is applicable. We may therefore state the following corollary.

Corollary 3.1.1: There exists a system of coordinates y^{*I}, $I=1,...,N$, in which an autonomous dynamical system

$$\dot{y}^A-\lambda^A(y)=0 \tag{3.7'}$$

takes the form

$$\dot{y}^{*A}-\delta^A_N=0. \tag{3.10'}$$

In the y^* coordinates the dynamical equations admit a symmetry mapping

$$\bar{y}^{*I}=y^{*I}+[N^{*(I)}(y^*,t)+\delta^I_N\eta^{*0}(y^*,t)]\delta a, \tag{3.11}$$

$$\bar{t}=t+\eta^{*0}(y^*,t)\delta a,\quad \eta^{*0}\ \text{arbitrary}, \tag{3.12}$$

where the functions $N^{*(I)}(y^*,t)$, $I=1,...,N$, are arbitrary constants of motion of (3.10'). ■

IV. CYCLIC VARIABLE SYMMETRY RELATIONS IN FIRST-ORDER SYSTEMS OBTAINED FROM SECOND-ORDER SYSTEMS

By a well-known procedure a system of n second-order ordinary differential equations may be reduced to an associated system of $N=2n$ first-order differential equations by defining $N=2n$ coordinates y^I by the relations

$$y^i\equiv x^i,\quad y^{i+n}\equiv\dot{x}^i,\quad i=1,...,n. \tag{4.1}$$

With reference to (2.1) and (3.1) it follows from (4.1) that

$$\lambda^i(y,t)\equiv y^{i+n}, \tag{4.2}$$

$$\lambda^{i+n}(y,t)=F^i(y^{j+n},y^j,t)=F^i(\dot{x}^i,x^i,t), \tag{4.3}$$

and hence when derived from the second-order system (2.1) the first-order system (3.1) specializes to the form

$$\dot{y}^i-y^{i+n}=0, \tag{4.4}$$

$$\dot{y}^{i+n}-F^i(y^{j+n},y^j,t)=0. \tag{4.5}$$

We examine this relationship between first- and second-order systems in order to determine how cyclic variables and concomitant special symmetries of a second-order system are affected by the above-mentioned reduction procedure. We also consider the applicability of Theorem 3.1 to those first-order systems derived from second-order systems with cyclic variables.

Consider first the case in which the second-order system (2.1) is cyclic in a coordinate x^r so that Theorem 2.1(b) is applicable. It then follows from (4.3)–(4.5) that the associated first-order system will be cyclic in the corresponding coordinate y^r, and hence Theorem 3.1 will be applicable.

Next consider the case in which a pair of variables $(x^s,\dot{x}^s)$ is cyclic in a second-order system (2.1), so that Theorem 2.1(a) is applicable. As in the previous case the coordinate y^s will still be cyclic in the associated first-order system (4.4) and (4.5). It is to be noted, however, that the presence of the coordinates y^{i+n}, $i=1,...,n$, in the n equations (4.4) precludes the possibility that any of the y^{i+n} could be cyclic in the associated first-order system (4.4) and (4.5). Thus Theorem 3.1 is applicable *only* for the cyclic coordinates y^s. Note, however, that the pair (y^s,y^{s+n}) will be

cyclic in the second half (4.5) of the first-order system (4.4) and (4.5).

When first- and second-order systems of differential equations are associated in the above-described manner their respective symmetry mapping functions $U^I(y,t)$ and $Z^i(\dot{x},x,t)$ [solutions, respectively, to (3.4) and (2.9)] will be related in that[2]

$$U^i(y,t) = Z^i(\dot{x},x,t), \tag{4.6}$$

$$U^{i+n}(y,t) \overset{0}{=} \dot{Z}^i(\dot{x},x,t). \tag{4.7}$$

Hence there will still be symmetry mappings of the first-order system (not described by Theorem 3.1) which are concomitant with a *pair* of cyclic variables $(x^s, \dot{x}^s)$ of the associated second-order system. To find these mappings we may use the symmetry functions $Z^i(\dot{x},x,t)$ [(2.23) and (2.24)] associated with the cyclic variables $(x^s, \dot{x}^s)$ of the second-order system and obtain by use of (4.6) and (4.7) the corresponding mapping functions $U^I(y,t)$ of the associated first-order system. These mapping functions are given in the following theorem.

Theorem 4.1: If a system of n second-order dynamical equations

$$\ddot{x}^i - F^i(\dot{x},x,t) = 0, \quad i,...,n, \tag{2.1'}$$

is cyclic in a pair of variables $(x^s, \dot{x}^s)$ in that $\partial F^i/\partial x^s = 0$ and $\partial F^i/\partial \dot{x}^s = 0$, then by the procedure of defining new variables $y^i \equiv x^i$, $y^{i+n} \equiv \dot{x}^i$, the second-order system (2.1') is reduced to the system of $N = 2n$ first-order equations

$$\dot{y}^i - y^{i+n} = 0, \tag{4.4'}$$

$$\dot{y}^{i+n} - F^i(y^{j+n}, y^j, t) = 0, \quad i,j = 1,...,n, \tag{4.5'}$$

where in (4.5') $\partial F^i/\partial y^s = 0$ and $\partial F^i/\partial y^{s+n} = 0$. This associated first-order system will admit an infinitesimal symmetry mapping

$$\bar{y}^I = y^I + [U^I(y,t) + \lambda^I(y,t)\eta^0(y,t)]\delta a, \quad I = 1,...,2n, \tag{3.2'}$$

$$\bar{t} = t + \eta^0(y,t)\delta a, \quad \eta^0(y,t) \text{ arbitrary}, \tag{3.3'}$$

where

$$\lambda^i(y,t) = y^{i+n}, \quad \lambda^{i+n}(y,t) = F^i(y^{j+n}, y^j, t) = F^i(\dot{x},x,t), \tag{4.8}$$

and where

$$U^s(y,t) = M^{(s)}(y,t)t + N^{(s)}(y,t), \tag{4.9}$$

$$U^{s+n}(y,t) = M^{(s)}(y,t), \tag{4.10}$$

$$U^I(y,t) = 0, \quad I \neq s \text{ or } s+n; \tag{4.11}$$

the functions $M^{(s)}(y,t)$ and $N^{(s)}(y,t)$ are arbitrary constants of motion of the first-order system (4.4') and (4.5'). ■

Remark 4.1: For the case $M^{(s)}(y,t) = 0$, Theorem 4.1 essentially reduces to a subcase of Theorem 3.1, for the cyclic variable y^s. ■

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[3] Unless indicated otherwise it is assumed that the functional notation $f(\dot{x},x,t)$ implies all variables $\dot{x}^i$ and x^i, $i = 1,...,n$, may be present.
[4] The notation "$\overset{t}{=}$" indicates equality when x^i, $\dot{x}^i$, $\ddot{x}^i$,... are expressed as functions of t and c^A by means of the solutions (2.2) and their derivatives.
[5] Repeated indices are to be summed over the index range. Lowercase Latin indices have the range 1,...,n, unless otherwise indicated. Uppercase Latin have the range 1,...,$2n$ or 1,...,N (as indicated), unless otherwise denoted.
[6] The notation "$\overset{0}{=}$" indicates equality when $\ddot{x}^i$ and higher dot derivatives are expressed as functions of $\dot{x}^i$, x^i, and t by means of the dynamical equations (2.1).
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Mean power reflection from a one-dimensional nonlinear random medium

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A model of wave propagation in a slab $0 \leqslant x \leqslant L$ of a *nonlinear random* medium is considered. The index of refraction is $k\,[1+\tilde{\epsilon}(x,w|u^{\epsilon}(x,L,w)|^2)]^{1/2}$, where $\tilde{\epsilon}(x,\alpha)=\epsilon m(x)+\epsilon^2[(n(x)+i\delta(x))\alpha+\theta(x)+i\gamma(x)]$, with ϵ a small parameter, m,n,δ,θ,γ suitable stochastic processes, $u^{\epsilon}(x,L,w)$ the wave field, and $w \geqslant 0$ the intensity of nonlinearity. The *mean reflected power* is evaluated from a certain nonlinear partial differential equation satisfied by the reflection coefficient $R^{\epsilon}(L,w)$. An infinite system of ordinary differential equations for the coefficients $R_n^{\epsilon}(L)$, $n=0,1,2,\ldots$, in the expansion of $R^{\epsilon}(L,w)$ in powers of w, is then derived, and the infinitesimal generator for the process $[R_0 R_0^* R_1 R_1^*]$, $R_n \equiv R_n^0(\epsilon^2 L)$, is obtained, in the *diffusion limit* $\epsilon \to 0$, $L \to \infty$, $\epsilon^2 L = \text{const}$. This allows us to compute $\langle |R|^2\rangle \cong \langle |R_0|^2\rangle + 2w\ \mathrm{Re}\langle R_0 R_1^*\rangle$ as a function of $\epsilon^2 L$. In the lossless case, $\delta=\gamma=0$, there is *no* correction due to the nonlinearity, in such a limit, and this remains true at least up to the order $O(w^2)$. Some effects can be observed when dissipation ($\delta>0$, $\gamma>0$) is taken into account. Numerical results are obtained and plots are given.

I. INTRODUCTION

Wave propagation in random media, that is in media whose properties are described only statistically, is of great interest in modeling several natural phenomena, e.g., in ocean acoustics and in optics of the atmosphere. Its analysis requires studying boundary-value (BV) problems for stochastic differential equations (see Refs. 1–3 for general references).

Some *linear stochastic* models have been studied in Refs. 1, 2, and 4–6, while the *nonlinear deterministic* case was considered in Refs. 7 and 8. However, propagation in *nonlinear random* media is important, for instance, in nonlinear optics and in electrodynamics of plasma. Therefore, the problem arises to investigate the joint effect of *both* nonlinearity *and* randomness.

Below we propose a one-dimensional model for this purpose. In the first approximation we consider the self-influence of a wave propagating through a plane-stratified slab of a random medium, as affecting the dielectric permittivity by its intensity, and neglect higher-order effects such as harmonics generation.

The paper is organized as follows. In Sec. II we transform the original two-point BV problem for the wave field, into an initial-value (IV) problem for a nonlinear partial differential equation (PDE) satisfied by the reflection coefficient $R^{\epsilon} \equiv R^{\epsilon}(L,w)$, L being the thickness of the slab, w the intensity of nonlinearity, and ϵ the size of the random fluctuations. An infinite system of ordinary differential equations (ODE's) is then obtained for the coefficients $R_n^{\epsilon}(L)$ in the expansion of $R^{\epsilon}(L,w)$ in powers of w. In Sec. III we compute the infinitesimal generator for the process solution $[R_0 R_0^* R_1 R_1^* \cdots R_N R_N^*]$, $R_n \equiv R_n^0(\epsilon^2 L)$, $n=0,1,\ldots,N$, of that system truncated at the $2(N+1)$th term, obtained in the *diffusion limit*. This is a limit that involves random perturbations of small size ϵ and large slab thicknesses L, as $\epsilon \to 0$, $L \to \infty$, with $\epsilon^2 L = \text{const}$. Indeed, many physical phenomena are affected by small random perturbations whose cumulative effects become important over long distances or time. Therefore such a limit provides a satisfactory description for several situations of physical interest (cf. Refs. 9 and 10).

In Sec. IV we compute the correction to the mean reflected power $E\{|R_0|^2\}$ of the linear problem ($w=0$), due to the nonlinearity. Various special cases such as the linear case itself with and without dissipation, as well as the nonlinear lossless problem, can be recovered from our more general analysis performed for the *nonlinear lossy* problem.

In Sec. V we report about the numerical treatment by which we evaluated the mean reflected power $E\{|R|^2\}$, in the general case. This program is carried out by solving numerically a certain system of *linear singular parabolic* equations. Various plots are given, correspondingly to several values of w and the loss parameters. In Sec. VI, finally, we summarize the results of the paper.

II. FORMULATION OF THE PROBLEM

Let $u^{\epsilon}(x,L,w)$ be the time-harmonic scalar wave field at location x, with the factor $e^{-i\omega_0 t}$ omitted. It satisfies the equations

$$u_{xx}^{\epsilon} + k^2[1+\tilde{\epsilon}(x,w|u^{\epsilon}(x,L,w)|^2)]u^{\epsilon}=0, \quad 0<x<L, \tag{2.1}$$

$$u^{\epsilon} = e^{-ik(x-L)} + R^{\epsilon}(L,w)e^{ik(x-L)}, \quad x>L, \tag{2.2}$$

$$u^{\epsilon} = T^{\epsilon}(L,w)e^{-ikx}, \quad x<0, \tag{2.3}$$

where k is the free-space (real-valued) wave number and the random medium is supposed to occupy a slab located between $x=0$ and $x=L$; $w \geqslant 0$ is the modulus square of the amplitude of the wave impinging on the slab, i.e., the intensity of nonlinearity; $R^{\epsilon}(L,w)$, $T^{\epsilon}(L,w)$ are the complex re-

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flection and transmission coefficients that characterize the scattering properties of the slab. The dependence on k will not be displayed.

The fluctuating part in the index of refraction has the form

$$\tilde{\epsilon}(x,\alpha) = \epsilon m(x) + \epsilon^2\{[n(x) + i\delta(x)]\alpha + \theta(x) + i\gamma(x)\}, \tag{2.4}$$

$\alpha \equiv w|u^\epsilon(x,L,w)|^2$, where ϵ is a small parameter characterizing the size of the fluctuations and $m(x)$, $n(x)$, $\delta(x)$, $\theta(x)$, $\gamma(x)$ are *real-valued almost surely bounded wide-sense stationary* stochastic processes, on an underlying probability space $(\Omega,\mathcal{A},P)$, with the dependence on the chance $\omega,\omega\in\Omega$, omitted, as usual. Here $E\{\cdot\}$ will denote taking expected values, i.e., integration over Ω, with respect to the measure P. Moreover, we assume that the processes above have the following properties.

(i) $m(x)$ is such that

$$E\{m(x)\} = 0, \quad E\{m(x)m(y)\} = \rho(|x-y|), \tag{2.5}$$

and satisfies a *strong mixing* condition, with mixing rate $\beta(T)$ such that $T^6\beta(T)\downarrow 0$ as $T\uparrow\infty$ (cf. Refs. 6 and 11).

(ii) $n(x)$, $\delta(x)$, $\gamma(x)$, $\theta(x)$ have constant (by stationarity), *nonzero means*,

$$E\{n(x)\} = \sigma, \quad \sigma = \text{const}, \quad E\{\delta(x)\} = \delta > 0, \quad E\{\gamma(x)\} = \gamma > 0, \quad E\{\theta(x)\} = \theta. \tag{2.5'}$$

In particular, such processes could be truly constant. The sign of δ,γ is chosen in view of the dependence $\sim e^{-i\omega_0 t}$, so that they represent *dissipation* (cf. Ref. 12 for the case of linear propagation in transmission lines; see also, Refs. 13–15 concerning nonlinear wave propagation in a deterministic lossy medium).

Under these conditions, $u^\epsilon(x,L,w)$, $R^\epsilon(L,w)$, and $T^\epsilon(L,w)$ also become stochastic processes and we are interested in studying the statistical properties of R^ϵ and T^ϵ. More precisely we are mainly concerned with the evaluation of the quantities $E\{|R^\epsilon|^2\}$, $E\{|T^\epsilon|^2\}$, because of their physical meaning of mean power reflected and transmitted, respectively, by the slab.

From the continuity of $u^\epsilon(x,L,w)$, $u_x^\epsilon(x,L,w)$ across the boundary of the slab, using (2.1)–(2.3), we obtain the boundary conditions for Eq. (2.1):

$$\begin{aligned} u^\epsilon(0,L,w) &= T^\epsilon(L,w), \\ u_x^\epsilon(0,L,w) &= -ikT^\epsilon(L,w) = -iku^\epsilon(0,L,w), \end{aligned} \tag{2.6}$$

$$\begin{aligned} u^\epsilon(L,L,w) &= 1 + R^\epsilon(L,w), \\ u_x^\epsilon(L,L,w) &= -ik[1 - R^\epsilon(L,w)] \\ &= -ik[2 - u^\epsilon(L,L,w)]. \end{aligned} \tag{2.7}$$

The BV problem [(2.1), (2.6), and (2.7)] is then equivalent to the integral equation

$$u^\epsilon(x,L,w) = e^{-ik(x-L)} + \frac{ik}{2}\int_0^L e^{ik|x-\xi|} \times \tilde{\epsilon}(\xi,w|u^\epsilon(\xi,L,w)|^2)u^\epsilon(\xi,L,w)d\xi \tag{2.8}$$

(cf. Refs. 1 and 8).

From (2.8) it is possible to obtain a nonlinear PDE satisfied by $R^\epsilon(L,w)$, with the advantage that the original BV problem is reduced to an IV problem. The technique used to attain such a result is referred to as "invariant imbedding." [1,8] We have

$$\frac{\partial R^\epsilon}{\partial L} = 2ikR^\epsilon + \frac{ik}{2}\tilde{\epsilon}(L,w|R^\epsilon + 1|^2)(R^\epsilon + 1)^2 + b\frac{\partial R^\epsilon}{\partial w}, \quad R^\epsilon(0,w) = 0, \tag{2.9}$$

where

$$b = w(a + a^*), \quad a = ik + \frac{ik}{2}\tilde{\epsilon}(L,w|R^\epsilon + 1|^2)(R^\epsilon + 1), \tag{2.10}$$

and $\tilde{\epsilon}(L,\alpha)$ is defined in (2.4).

In the linear case ($w = 0$), (2.9) reduces to a Riccati differential equation [cf. Ref. 6, formula (2.7); Ref. 1, formula (7)].

Hereafter, we drop the label ϵ. Assume that $R(L,w)$ can be expanded in powers of w:

$$R(L,w) = \sum_{r=0}^{\infty} R_r(L)\frac{w^r}{r!}, \quad R_r(L) \equiv \frac{\partial^r R(L,w)}{\partial w^r}\bigg|_{w=0}, \tag{2.11}$$

and transform (2.9) into an infinite-dimensional system of ODE's for the $R_r(L)$'s. For simplicity, we shall confine ourselves to within the order $O(w)$, as we are interested in computing the first correction to the linear case, due to nonlinearity. Therefore we just write

$$R(L,w) = R_0(L) + wR_1(L) + O(w^2) \tag{2.12}$$

in (2.9). Something about the order $O(w^2)$ will be stated below, in Sec. IV. We obtain, after a little algebra and equating the quantities independent of w, and the coefficients of w:

$$\begin{aligned} \frac{dR_0}{dL} &= 2ikR_0 + \frac{ik}{2}\epsilon m(R_0+1)^2 + \frac{ik}{2}\epsilon^2(\theta + i\gamma)(R_0+1)^2, \\ \frac{dR_1}{dL} &= 2ikR_1 + k\epsilon m\left[i(R_0+1) - \left(\frac{R_0 - R_0^*}{2i}\right)\right]R_1 + k\epsilon^2\left\{\frac{1}{2}(in-\delta)|R_0+1|^2(R_0+1)^2\right. \\ &\quad \left. + \left[(i\theta-\gamma)(R_0+1) - \theta\left(\frac{R_0-R_0^*}{2i}\right) - \gamma\left(\frac{R_0+R_0^*}{2}\right) - \gamma\right]R_1\right\}, \end{aligned} \tag{2.13}$$

with the initial values

$$R_0(0)=0, \quad R_1(0)=0. \tag{2.13'}$$

Note that $R_0(L)$ is the reflection coefficient in the linear case.

System (2.13) can be given a more standard form, by setting

$$R_r \equiv z_r e^{i\alpha}, \quad \alpha \equiv 2kL \quad (\text{real}), \quad r=0,1, \tag{2.14}$$

to "remove" the $O(1)$ terms on the right-hand side. We obtain

$$\begin{aligned}
\frac{dz_0}{dL} &= \frac{ik}{2}\epsilon m(z_0 e^{ikL}+e^{-ikL})^2+\frac{ik}{2}\epsilon^2(\theta+i\gamma)(z_0e^{ikL}+e^{-ikL})^2,\\
\frac{dz_1}{dL} &= \frac{ik}{2}\epsilon m(3z_0e^{2ikL}-z_0^* e^{-2ikL}+2)z_1+\frac{k\epsilon^2}{2}\{(in-\delta)[z_0^2(3+z_0z_0^*)e^{2ikL}+z_0^3e^{4ikL}\\
&\quad +3z_0(1+z_0z_0^*)+(1+3z_0z_0^*)e^{-2ikL}+z_0^*e^{-4ikL}]\\
&\quad +[3(i\theta-\gamma)z_0e^{2ikL}-(i\theta+\gamma)z_0^*e^{-2ikL}+2(i\theta-2\gamma)]z_1\},
\end{aligned} \tag{2.15}$$

with the initial values

$$z_0(0)=0, \quad z_1(0)=0. \tag{2.15'}$$

III. DIFFUSION LIMIT

Instead of separating real and imaginary parts in (2.15), it is convenient to use *complex notation* (cf. Ref. 9). If we denote complex conjugate quantities by an asterisk, we get, with obvious positions, the system of four ODE's

$$\begin{aligned}
\frac{dz_0}{dL} &= \epsilon m F_0+\epsilon^2 H_0,\\
\frac{dz_0^*}{dL} &= \epsilon m F_0^*+\epsilon^2 H_0^*,\\
\frac{dz_1}{dL} &= \epsilon m F_1+\epsilon^2(nG_1+H_1),\\
\frac{dz_1^*}{dL} &= \epsilon m F_1^*+\epsilon^2(nG_1^*+H_1^*),
\end{aligned} \tag{3.1}$$

with the initial values

$$z_0(0)=z_0^*(0)=0, \quad z_1(0)=z_1^*(0)=0. \tag{3.1'}$$

Note that H_0, H_1 *include* the dissipative terms ($H_0\equiv 0$, $H_1\equiv 0$, when $\delta=\gamma=\theta=0$).

For short, we write (3.1) as

$$\frac{d\zeta^\epsilon}{dL}=\epsilon m\Phi+\epsilon^2(n\Gamma+\Lambda), \tag{3.2}$$

where

$$\begin{aligned}
\zeta^\epsilon &\equiv (\zeta_i)_{i=1,\dots,4}\equiv[z_0\, z_0^*\, z_1\, z_1^*]^T,\\
\Phi &\equiv (\Phi_i)_{i=1,\dots,4}\equiv[F_0\, F_0^*\, F_1\, F_1^*]^T,\\
\Gamma &\equiv (\Gamma_i)_{i=1,\dots,4}\equiv[0\,0\,G_1\,G_1^*]^T,\\
\Lambda &\equiv (\Lambda_i)_{i=1,\dots,4}\equiv[H_0\,H_0^*\,H_1\,H_1^*]^T.
\end{aligned} \tag{3.3}$$

Therefore

$$\zeta_{2r+1}\equiv z_r, \quad \zeta_{2r+2}\equiv z_r^* \tag{3.4}$$

$$\Phi_{2r+1}\equiv F_r, \quad \Phi_{2r+2}\equiv F_r^* \quad (r=0,1), \tag{3.5}$$

and similarly for the Γ_r's and the Λ_r's.

System (3.2) is in a suitable form for us to apply the Kahsminskii theorem to determine the diffusion matrix and the drift vector associated with the stochastic process $\zeta(\cdot)\equiv\zeta^0(\cdot)$ obtained in the limit $\epsilon\to 0$, $L\to+\infty$, with $\epsilon^2 L=\text{const}$ (*diffusion limit*) (see Refs. 6, 11, and 16). We have to compute the quantities

$$\begin{aligned}
a_{ij}(\zeta) &\equiv \lim_{T\uparrow\infty}\frac{1}{T}\int_{t_0}^{t_0+T}\int_{t_0}^{s}\rho(s-\sigma)\Phi_i(\zeta,s)\\
&\quad\times\Phi_j(\zeta,\sigma)\,d\sigma\,ds, \quad i,j=1,\dots,4,
\end{aligned} \tag{3.6}$$

$$\begin{aligned}
b_i(\zeta) &\equiv \lim_{T\uparrow\infty}\frac{1}{T}\int_{t_0}^{t_0+T}\int_{t_0}^{s}\rho(s-\sigma)\\
&\quad\times\sum_{j=1}^{4}\frac{\partial\Phi_i(\zeta,s)}{\partial\zeta_j}\Phi_j(\zeta,\sigma)\,d\sigma\,ds, \quad i=1,\dots,4,
\end{aligned} \tag{3.7}$$

$$\begin{aligned}
d_i(\zeta) &\equiv c_i(\zeta)+\Delta c_i(\zeta),\\
c_i(\zeta) &\equiv \lim_{T\uparrow\infty}\frac{1}{T}\int_{t_0}^{t_0+T}\sigma\,\Gamma_i(\zeta,s)\,ds \quad (\sigma\equiv E\{n(x)\}),
\end{aligned} \tag{3.8}$$

$$\Delta c_i(\zeta)\equiv\lim_{T\uparrow\infty}\frac{1}{T}\int_{t_0}^{t_0+T}E\{\Lambda_i(\zeta,s)\}ds, \quad i=1,\dots,4.$$

Note that $c_1\equiv 0$, $c_2\equiv 0$, being $\Gamma_1\equiv 0$, $\Gamma_2\equiv 0$. The parameters δ,θ,γ appear only in the quantities Δc_i's and therefore affect only the drift.

The integrals in (3.6)–(3.8) have to exist uniformly in ζ, t_0. The assumed stationarity for the processes permits us to set $t_0=0$.

It is convenient to display the dependence of Φ,Γ,Λ on L. From (3.1) and (2.15) we obtain

$$\begin{aligned}
F_r(L) &\equiv i(k/2)[\alpha_r e^{i\alpha}+\beta_r e^{-i\alpha}+2z_r],\\
G_r(L) &\equiv i(k/2)[\gamma_r e^{i\alpha}+\delta_r e^{-i\alpha}+\epsilon_r+\eta_r e^{2i\alpha}\\
&\quad +\theta_r e^{-2i\alpha}] \quad (\alpha\equiv 2kL, \quad r=0,1),
\end{aligned} \tag{3.9}$$

where

$$\alpha_0 = z_0^2, \quad \beta_0 = 1, \tag{3.10}$$
$$\gamma_0 = \delta_0 = \epsilon_0 = \eta_0 = \theta_0 = 0;$$
$$\alpha_1 = 3z_0 z_1 = 3\zeta_1\zeta_3, \quad \beta_1 = -z_0^* z_1 = -\zeta_2\zeta_3,$$
$$\gamma_1 = z_0^2(3 + z_0 z_0^*) = \zeta_1^2(3 + \zeta_1\zeta_2),$$
$$\delta_1 = 1 + 3z_0 z_0^* = 1 + 3\zeta_1\zeta_2, \tag{3.11}$$
$$\epsilon_1 = 3z_0(1 + z_0 z_0^*) = 3\zeta_1(1 + \zeta_1\zeta_2),$$
$$\eta_1 = z_0^3 = \zeta_1^3, \quad \theta_1 = z_0^* = \zeta_2.$$

Let us first compute the quantities $\Phi_i(x)\Phi_j(x-y)$, $[\partial\Phi_i(x)/\partial\zeta_j]\Phi_j(x-y)$ (the dependence on ζ has been dropped, for short). The long though elementary calculations will be omitted. The structure of these quantities is as follows:

$$\Phi_i(x)\Phi_j(x-y) \equiv -(k^2/4)[\phi_1^{ij}(x)e^{iy} + \phi_2^{ij}(x)e^{-iy} + \phi_3^{ij}(x)], \tag{3.12}$$

and

$$\frac{\partial\Phi_i(x)}{\partial\zeta_j}\Phi_j(x-y) = -(k^2/4)[\psi_1^{ij}(x)e^{iy} + \psi_2^{ij}(x)e^{-iy} + \psi_3^{ij}(x)], \tag{3.13}$$

where $\phi_k^{ij}(x)$ and $\psi_k^{ij}(x)$ are certain functions of x. More precisely, they are linear functions of $e^{\pm ix}$, $e^{\pm 2ix}$, with coefficients depending on the ζ_i's.

Now we can compute the diffusion matrix and the drift vector. By using (3.12) in (3.6), we have, for $i,j = 1,...,4$,

$$a_{ij}(\zeta) \equiv \lim_{T\uparrow\infty}\frac{1}{T}\int_{t_0}^{t_0+T}\int_{t_0}^{s}\rho(s-\sigma)\Phi_i(s)\Phi_j(\sigma)\,ds\,d\sigma$$
$$\equiv \lim_{T\uparrow\infty}(1/T)I_{ij}(T), \tag{3.14}$$

$$I_{ij}(T) = \frac{1}{4k^2}\int_0^{2kT}\int_0^{x}\tilde\rho(y)\Phi_i(x)\Phi_j(x-y)\,dx\,dy$$
$$= -\frac{1}{16}\left\{\int_0^{2kT}\tilde\rho(y)e^{iy}\left(\int_y^{2kT}\phi_1^{ij}(x)dx\right)dy + \int_0^{2kT}\tilde\rho(y)e^{-iy}\left(\int_y^{2kT}\phi_2^{ij}(x)dx\right)dy + \int_0^{2kT}\tilde\rho(y)\left(\int_y^{2kT}\phi_3^{ij}(x)dx\right)dy\right\}. \tag{3.15}$$

Here we used the stationarity of $m(\cdot)$ to set $t_0 = 0$ and the same letter Φ_i after changing $2ks$ in $s[\equiv x]$; $\tilde\rho(y) \equiv \rho(y/2k)$ and the order of integration has been changed.

At this point we observed that *only* the terms *constant* with x in $\phi_k^{ij}(x)$, $k = 1,2,3$, play a role. In fact, the exponentials give contributions, after integration, which are *bounded* for $T\in[0,\infty)$. Thus, in view of the limit in (3.14), we just need to write

$$\int_y^{2kT}\phi_k^{ij}(x)dx \equiv \chi_k^{ij}(2kT - y) + (\cdots), \quad k = 1,2,3, \tag{3.16}$$

where dots denote T-bounded quantities and

$$\chi_1^{ij} = \begin{cases}\alpha_{(i-1)/2}\beta_{(j-1)/2}, & i,j = 1,3,\\ -\alpha_{(i-1)/2}\alpha^*_{j/2-1}, & i = 1,3, \quad j = 2,4,\\ -\beta^*_{i/2-1}\beta_{(j-1)/2}, & i = 2,4, \quad j = 1,3,\\ \beta^*_{i/2-1}\alpha^*_{j/2-1}, & i,j = 2,4;\end{cases}$$
$$\chi_2^{ij} = \begin{cases}\beta_{(i-1)/2}\alpha_{(j-1)/2}, & i,j = 1,3,\\ -\beta_{(i-1)/2}\beta^*_{j/2-1}, & i = 1,3, \quad j = 2,4,\\ -\alpha^*_{i/2-1}\alpha_{(j-1)/2}, & i = 2,4, \quad j = 1,3,\\ \alpha^*_{i/2-1}\beta^*_{j/2-1}, & i,j = 2,4;\end{cases} \tag{3.17}$$
$$\chi_3^{ij} = \begin{cases}4z_{(i-1)/2}z_{(j-1)/2}, & i,j = 1,3,\\ -4z_{(i-1)/2}z^*_{j/2-1}, & i = 1,3, \quad j = 2,4,\\ -4z^*_{i/2-1}z_{(j-1)/2}, & i = 2,4, \quad j = 1,3,\\ 4z^*_{i/2-1}z^*_{j/2-1}, & i,j = 2,4.\end{cases}$$

Hence, we obtain from (3.14) and (3.15)

$$a_{ij}(\zeta) = \lim_{T\uparrow\infty}(1/T)I_{ij}(T)$$
$$= -\frac{k^2}{4}\left\{\chi_1^{ij}\int_0^{+\infty}\rho(\tau)e^{2ik\tau}\,d\tau + \chi_2^{ij}\int_0^{+\infty}\rho(\tau)e^{-2ik\tau}\,d\tau + \chi_3^{ij}\int_0^{+\infty}\rho(\tau)d\tau\right\}.$$

Here we have taken into account the mixing property of $m(\cdot)$, which entails

$$\left|\int_0^{2kT} y\,\tilde\rho(y)dy\right| < \int_0^{+\infty} y\,\tilde\rho(y)dy < \infty$$

[cf. (i) and Ref. 11]. We conclude that

$$a_{ij}(\zeta) = -(k^2/4)[\chi_1^{ij}J_1 + \chi_2^{ij}J_2 + \chi_3^{ij}J_3], \quad i,j = 1,...,4, \tag{3.18}$$

where

$$J_1 \equiv \int_0^{+\infty}\rho(\tau)e^{2ik\tau}\,d\tau,$$
$$J_2 \equiv \int_0^{+\infty}\rho(\tau)e^{-2ik\tau}\,d\tau, \tag{3.19}$$
$$J_3 \equiv \int_0^{+\infty}\rho(\tau)d\tau.$$

Proceeding in a similar way, we can compute $b_i(\zeta)$ from (3.7). Recalling (3.13) we have immediately

$$b_i(\zeta) = -\frac{1}{16}\lim_{T\uparrow\infty}\frac{1}{T}\left\{\int_0^{2kT}\int_y^{2kT}\tilde\rho(y) \times\sum_{j=1}^{4}[\psi_1^{ij}(x)e^{iy} + \psi_2^{ij}(x)e^{-iy} + \psi_3^{ij}(x)]\,dx\,dy\right\}. \tag{3.20}$$

Analogously to what has been done in (3.16) for the $\phi_k^{ij}(x)$, $k=1,2,3$, let us denote by Θ_k^{ij}, $k=1,2,3$, the terms in $\psi_k^{ij}(x)$ that are constant with x. We obtain

$$\int_y^{2kT} \psi_k^{ij}(x)dx = \Theta_k^{ij}(2kT-y) + (\cdots)\,,$$
$$i,j=1,\ldots,4, \quad k=1,2,3\,, \tag{3.21}$$

where

$$\Theta_1^{ij} = \begin{cases} A_{(i-1)/2,j}\beta_{(j-1)/2}, & i,j=1,3,\\ -A_{(i-1)/2,j}\alpha^*_{j/2-1}, & i=1,3, \quad j=2,4,\\ -E_{i/2-1,j}\beta_{(j-1)/2}, & i=2,4, \quad j=1,3,\\ E_{i/2-1,j}\alpha^*_{j/2-1}, & i,j=2,4\,; \end{cases}$$

$$\Theta_2^{ij} = \begin{cases} B_{(i-1)/2,j}\alpha_{(j-1)/2}, & i,j=1,3,\\ -B_{(i-1)/2,j}\beta^*_{j/2-1}, & i=1,3, \quad j=2,4,\\ -D_{i/2-1,j}\alpha_{(j-1)/2}, & i=2,4, \quad j=1,3,\\ D_{i/2-1,j}\beta^*_{j/2-1}, & i,j=2,4\,; \end{cases} \tag{3.22}$$

$$\Theta_3^{ij} = \begin{cases} 2C_{(i-1)/2,j}z_{(j-1)/2}, & i,j=1,3,\\ -2C_{(i-1)/2,j}z^*_{j/2-1}, & i=1,3, \quad j=2,4,\\ -2F_{i/2-1,j}z_{(j-1)/2}, & i=2,4, \quad j=1,3,\\ 2F_{i/2-1,j}z^*_{j/2-1}, & i,j=2,4\,; \end{cases}$$

where

$$A_{ij}\equiv\frac{\partial\alpha_i}{\partial\zeta_j}, \quad B_{ij}\equiv\frac{\partial\beta_i}{\partial\zeta_j}, \quad C_{ij}\equiv 2\frac{\partial z_i}{\partial\zeta_j},$$
$$D_{ij}\equiv\frac{\partial(\alpha_i^*)}{\partial\zeta_j}, \quad E_{ij}\equiv\frac{\partial(\beta_i^*)}{\partial\zeta_j}, \quad F_j\equiv 2\frac{\partial(z_i^*)}{\partial\zeta_j}. \tag{3.23}$$

Only these quantities contribute to $b_i(\zeta)$. We obtain

$$b_i(\zeta) = -\frac{k^2}{4}\Big[J_1\Big(\sum_{j=1}^4\Theta_1^{ij}\Big) + J_2\Big(\sum_{j=1}^4\Theta_2^{ij}\Big) + J_3\Big(\sum_{j=1}^4\Theta_3^{ij}\Big)\Big], \quad i=1,\ldots,4\,, \tag{3.24}$$

with J_k, $k=1,2,3$, defined in (3.19).

From (3.8), (3.3), and (2.15),

$$c_i(\zeta) = \begin{cases} = \lim_{T\uparrow\infty}\frac{1}{T}\int_0^T \sigma\, G_{(i-1)/2}(s)ds, & i=3,\\ = \lim_{T\uparrow\infty}\frac{1}{T}\int_0^T \sigma\, G^*_{i/2-1}(s)ds, & i=4. \end{cases} \tag{3.25}$$

Recall that $\Gamma_1\equiv 0$, $\Gamma_2\equiv 0$. Thus $c_1\equiv 0$, $c_2\equiv 0$. By using (3.9), we have

$$c_3(\zeta) = i\frac{k}{2}\lim_{T\uparrow\infty}\frac{1}{T}\int_0^{2kT}\sigma[\gamma_1 e^{2ikx} + \delta_1 e^{-2ikx} + \epsilon_1 + \eta_1 e^{4ikx} + \theta_1 e^{-4ikx}]dx\,, \tag{3.26}$$
$$c_4(\zeta) = c_3^*(\zeta)\,.$$

Suppose $\sigma\neq 0$ [cf. (2.5′)]. Then

$$c_3(\zeta) = i(k/2)\sigma\,\epsilon_1\,, \tag{3.27}$$

with ϵ_1 defined in (3.11).

Finally, recalling that, from (2.15), (3.1), and (3.3),

$$\Lambda_1\equiv H_0 = (ik/2)(\theta+i\gamma)(z_0e^{ikL}+e^{-ikL})^2\,,$$
$$\Lambda_3\equiv H_1 = (k/2)\{-\delta[z_0^2(3+z_0z_0^*)e^{2ikL} + z_0^3e^{4ikL} + 3z_0(1+z_0z_0^*) + (1+3z_0z_0^*)e^{-2ikL} + z_0^*e^{-4ikL}] + [3(i\theta-\gamma)z_0e^{2ikL} - (i\theta+\gamma)z_0^*e^{-2ikL} + 2(i\theta-2\gamma)]z_1\}\,, \tag{3.28}$$
$$\Lambda_2 = \Lambda_1^*, \quad \Lambda_4 = \Lambda_3^*\,,$$

we obtain from (3.8) and (2.5′), by an easy calculation,

$$\Delta c_1 = k(i\theta-\gamma)z_0, \quad \Delta c_3 = -\tfrac{1}{2}k\delta z_0(1+z_0z_0^*) + k(i\theta-2\gamma)z_1\,, \tag{3.29}$$

while $\Delta c_2 = (\Delta c_1)^*$, $\Delta c_4 = (\Delta c_3)^*$.

All computations in this section yield the *infinitesimal generator*

$$L_N\equiv\sum_{i,j=1}^{2N+2}a_{ij}(\zeta)\frac{\partial^2}{\partial\zeta_i\partial\zeta_j} + \sum_{i=1}^{2N+2}[b_i(\zeta)+d_i(\zeta)]\frac{\partial}{\partial\zeta_i}, \tag{3.30}$$

with $a_{ij}(\zeta)$, $b_i(\zeta)$, $d_i(\zeta)$ given by (3.18), (3.17), (3.19), (3.24) and (3.8), (3.29), (3.27). Actually we confined ourselves to $N=1$, which corresponds to the statistical description of system (2.13) for R_0, R_1. For $N=0$ we recover the *linear* problem ($w=0$), corresponding to the Riccati equation for R_0, which appears in (2.13). The general case of $N\geqslant 2$ refers to the larger system for $R_0, R_0^*, R_1, R_1^*,\ldots,R_N, R_N^*$ that we did not work out.

It is convenient to decompose the (linear) operator L_N into the sum

$$L_N\equiv\mathscr{L}+\mathscr{M}_N+\mathscr{N}_N\,, \tag{3.31}$$

where $\mathscr{L}$, $\mathscr{M}_N$, $\mathscr{N}_N$ are linear operators, with $\mathscr{L}$ acting *only* on ζ_1,ζ_2 and $\mathscr{N}_N$ acting *only* on $\zeta_{2N+1},\zeta_{2N+2}$:

$$\mathscr{L}\equiv a_{11}\frac{\partial^2}{\partial\zeta_1^2} + (a_{12}+a_{21})\frac{\partial^2}{\partial\zeta_1\partial\zeta_2} + a_{22}\frac{\partial^2}{\partial\zeta_2^2} + (b_1+d_1)\frac{\partial}{\partial\zeta_1} + (b_2+d_2)\frac{\partial}{\partial\zeta_2}\,. \tag{3.32}$$

Here $d_i=\Delta c_i$, $i=1,2$, as $c_i=0$ for $i=1,2$;

$$\mathcal{N}_N \equiv a_{2N+1,2N+1}\frac{\partial^2}{\partial\xi_{2N+1}^2} + (a_{2N+1,2N+2} + a_{2N+2,2N+1})\frac{\partial^2}{\partial\xi_{2N+1}\partial\xi_{2N+2}}$$
$$+ a_{2N+2,2N+2}\frac{\partial^2}{\partial\xi_{2N+2}^2} + (b_{2N+1} + d_{2N+1})\frac{\partial}{\partial\xi_{2N+1}} + (b_{2N+2} + d_{2N+2})\frac{\partial}{\partial\xi_{2N+2}}; \tag{3.33}$$

$$\mathcal{M}_N \equiv \sum_{i,j=3}^{2N} a_{ij}\frac{\partial^2}{\partial\xi_i\partial\xi_j} + \sum_{i=1}^{2N}(b_i + d_i)\frac{\partial}{\partial\xi_i} + \sum_{i=3}^{2N+2}(a_{i,1} + a_{1,i})\frac{\partial^2}{\partial\xi_1\partial\xi_i} + \sum_{i=3}^{2N+2}(a_{i,2} + a_{2,i})\frac{\partial^2}{\partial\xi_2\partial\xi_i}$$
$$+ \sum_{i=3}^{2N}(a_{i,2N+1} + a_{2N+1,i})\frac{\partial^2}{\partial\xi_i\partial\xi_{2N+1}} + \sum_{i=3}^{2N}(a_{i,2N+2} + a_{2N+2,i})\frac{\partial^2}{\partial\xi_i\partial\xi_{2N+2}}. \tag{3.34}$$

IV. THE CORRECTION DUE TO NONLINEARITY

From the expansion (2.13) for $R(L,w)$, we obtain

$$|R|^2 = RR^* = |R_0|^2 + 2w\,\mathrm{Re}(R_0 R_1^*) + O(w^2)\,. \tag{4.1}$$

Recalling (2.15), we have also $R_0 R_1^* = z_0 z_1^*$, as α is real. Therefore,

$$E\{|R|^2\} = E\{|R_0|^2\} + 2w\,\mathrm{Re}\,E\{R_0 R_1^*\} + O(w^2)$$
$$= E\{|z_0|^2\} + 2w\,\mathrm{Re}\,E\{z_0 z_1^*\} + O(w^2)\,. \tag{4.2}$$

Here $|R|^2$ represents the power reflected from the slab and $E\{|R|^2\}$ its *mean* value. When $w = 0$, we recover the corresponding quantities for the *linear* problem, $|R_0|^2$ and $E\{|R_0|^2\}$ (cf. Ref. 6).

In this section we shall compute the first correction to $E\{|R_0|^2\}$ due to the nonlinearity, as given in (4.2).

Consider the problem

$$U_\tau = L_1[U] \quad \left(U_\tau \equiv \frac{\partial U}{\partial\tau}\right),$$
$$U|_{\tau=0} = \zeta_1\zeta_2 + w(\zeta_1\zeta_4 + \zeta_2\zeta_3)\,, \tag{4.3}$$

for $U \equiv U(\zeta_1,\zeta_2,\zeta_3,\zeta_4;\tau)$, $\tau \equiv \epsilon^2 L$, the operator L_1 being given by (3.30) for $N = 1$. Note that

$$\zeta_1\zeta_2 + w(\zeta_1\zeta_4 + \zeta_2\zeta_3) = z_0 z_0^* + w(z_0 z_1^* + z_0^* z_1)$$
$$= |R_0|^2 + 2w\,\mathrm{Re}(R_0 R_1^*)\,.$$

Therefore, the solution to (4.3) will enable us to calculate

$$E\{|R_0|^2\} + 2w\,\mathrm{Re}(R_0 R_1^*) = U(0,0,0,0;\tau) \tag{4.4}$$

as a function of $\tau \equiv \epsilon^2 L$, i.e., the mean reflected power, approximated up to the order $O(w)$.

To solve (4.3), we set, as an ansatz,

$$U(\zeta_1,\zeta_2,\zeta_3,\zeta_4;\tau)$$
$$= \mathcal{A}(\zeta_1,\zeta_2;\tau) + \mathcal{B}(\zeta_1,\zeta_2;\tau)\zeta_3 + \mathcal{C}(\zeta_1,\zeta_2;\tau)\zeta_4\,. \tag{4.5}$$

The initial condition in (4.3), considered as an *identity* in ζ_3,ζ_4, entails

$$\mathcal{A}(\zeta_1,\zeta_2;0) = \zeta_1\zeta_2\,,$$
$$\mathcal{B}(\zeta_1,\zeta_2;0) = w\zeta_2\,, \tag{4.6}$$
$$\mathcal{C}(\zeta_1,\zeta_2;0) = w\zeta_1\,.$$

Substitution of (4.5) in (4.3) yields [denoting now by $\mathcal{M}$ the operator $\mathcal{M}_1 + \mathcal{N}_1$ in (3.31)]

$$U_\tau = \mathcal{A}_\tau + \mathcal{B}_\tau\zeta_3 + \mathcal{C}_\tau\zeta_4$$
$$= L_1[\mathcal{A}] + L_1[\mathcal{B}\zeta_3] + L_1[\mathcal{C}\zeta_4]$$
$$= \mathcal{L}[\mathcal{A}] + \mathcal{L}[\mathcal{B}]\zeta_3 + \mathcal{L}[\mathcal{C}]\zeta_4$$
$$+ \mathcal{M}[\mathcal{B}\zeta_3] + \mathcal{M}[\mathcal{C}\zeta_4]\,, \tag{4.7}$$

because $\mathcal{A}$ is *independent* of ζ_3,ζ_4 (and therefore $\mathcal{M}[\mathcal{A}] \equiv 0$) and $\mathcal{L}$ does *not* act on ζ_3,ζ_4 (and therefore $\mathcal{L}[\mathcal{B}\zeta_3] = \mathcal{L}[\mathcal{B}]\zeta_3$, $\mathcal{L}[\mathcal{C}\zeta_4] = \mathcal{L}[\mathcal{C}]\zeta_4$). From (3.33) and (3.34) we obtain

$$\mathcal{N}_1 = a_{33}\frac{\partial^2}{\partial\zeta_3^2} + (a_{34} + a_{43})\frac{\partial^2}{\partial\zeta_3\partial\zeta_4}$$
$$+ a_{44}\frac{\partial^2}{\partial\zeta_4^2} + (b_3 + d_3)\frac{\partial}{\partial\zeta_3} + (b_4 + d_4)\frac{\partial}{\partial\zeta_4}, \tag{4.8}$$

$$\mathcal{M}_1 = \sum_{i=3}^{4}(a_{i,1} + a_{1,i})\frac{\partial^2}{\partial\zeta_1\partial\zeta_i} + \sum_{i=3}^{4}(a_{i,2} + a_{2,i})\frac{\partial^2}{\partial\zeta_2\partial\zeta_i}$$
$$= (a_{13} + a_{31})\frac{\partial^2}{\partial\zeta_1\partial\zeta_3} + (a_{14} + a_{41})\frac{\partial^2}{\partial\zeta_1\partial\zeta_4}$$
$$+ (a_{23} + a_{32})\frac{\partial^2}{\partial\zeta_2\partial\zeta_3} + (a_{24} + a_{42})\frac{\partial^2}{\partial\zeta_2\partial\zeta_4}. \tag{4.9}$$

Therefore

$$\mathcal{M}[\mathcal{B}\zeta_3] \equiv \mathcal{N}_1[\mathcal{B}\zeta_3] + \mathcal{M}_1[\mathcal{B}\zeta_3]$$
$$= (b_3 + d_3)\mathcal{B} + (a_{13} + a_{31})\frac{\partial\mathcal{B}}{\partial\zeta_1}$$
$$+ (a_{23} + a_{32})\frac{\partial\mathcal{B}}{\partial\zeta_2},$$
$$\mathcal{M}[\mathcal{C}\zeta_4] \equiv \mathcal{N}_1[\mathcal{C}\zeta_4] + \mathcal{M}_1[\mathcal{C}\zeta_4]$$
$$= (b_4 + d_4)\mathcal{C} + (a_{14} + a_{41})\frac{\partial\mathcal{C}}{\partial\zeta_1}$$
$$+ (a_{24} + a_{42})\frac{\partial\mathcal{C}}{\partial\zeta_2}. \tag{4.10}$$

In order to obtain a system of PDE's for $\mathcal{A}$, $\mathcal{B}$, $\mathcal{C}$ from (4.7), considered as an identity in ζ_3, ζ_4, we have to display the dependence of a_{ij}, b_i, and d_i on the ζ's. To contain the lengthy and cumbersome calculations we have to perform to

get such coefficients, observe that the quantities χ_k^{ij} $(i,j=1,2,...,2N+2,\ k=1,2,3)$, defined in (3.17), enjoy the properties

$$\chi_1^{ij}=\chi_2^{ji},\quad \chi_3^{ij}=\chi_3^{ji},\quad i,j=1,2,...,2N+2\,, \tag{4.11}$$

and thus

$$\begin{aligned} a_{ii} &= -\frac{k^2}{2}I_1\left(\chi_1^{ii}+\frac{r_{31}}{4}\chi_3^{ii}\right),\quad i=1,2,...,2N+2\,,\\ a_{ij}+a_{ji} &= -\frac{k^2}{2}I_1\left[(\chi_1^{ij}+\chi_1^{ji})+\frac{r_{31}}{2}\chi_3^{ij}\right],\\ & i,j=1,2,...,2N+2\,, \end{aligned} \tag{4.12}$$

where

$$\begin{aligned} I_1 &\equiv \int_0^{+\infty}\rho(\tau)\cos 2k\tau\, d\tau,\\ I_2 &\equiv \int_0^{+\infty}\rho(\tau)\sin 2k\tau\, d\tau\,,\\ I_3 &\equiv 2\int_0^{+\infty}\rho(\tau)d\tau\,, \end{aligned} \tag{4.13}$$

and $r_{31}\equiv I_3/I_1$. Essentially, I_1 is the *power spectral density* of the process $m(\cdot)$ [cf. (2.5)].

As for the b_i's, setting

$$\begin{aligned} b_i^{(N)} \equiv -\frac{k^2}{4}\Bigg[J_1\Bigg(\sum_{j=1}^{2N+2}\Theta_1^{ij}\Bigg)+J_2\Bigg(\sum_{j=1}^{2N+2}\Theta_2^{ij}\Bigg)\\ +J_3\Bigg(\sum_{j=1}^{2N+2}\Theta_3^{ij}\Bigg)\Bigg],\quad i=1,2,...,2N+2\,, \end{aligned} \tag{4.14}$$

we have, for each integer $N\geqslant 1$,

$$b_i^{(N+1)}=b_i^{(N)}\,, \tag{4.15}$$

for $1\leqslant i\leqslant 2N+2$. In other words,

$$\Theta_k^{ij}=0\,, \tag{4.16}$$

for $i=1,2,...,2N+2$, $k=1,2,3$, *if* $j>2N+2$, i.e., passing from a given degree of approximation to the following, the components of the drift vector previously computed are *unchanged* at the new stage.

Let us first compute the coefficients of the operator $\mathscr{L}$, i.e., that one describing the *linear* problem $(w=0)$. Using (3.10) we have $\alpha_0=z_0^2=\zeta_1^2$, $\beta_0=1$ and hence $\alpha_0^*=z_0^{*2}=\zeta_2^2$, $\beta_0^*=1$, and, from (3.17) and (3.22),

$$\begin{aligned} &\chi_1^{11}=\zeta_1^2,\quad \chi_1^{12}=-\zeta_1^2\zeta_2^2\,,\\ &\chi_1^{21}=-1,\quad \chi_1^{22}=\zeta_2^2\,,\\ &\chi_3^{11}=4\zeta_1^2,\quad \chi_3^{12}=-4\zeta_1\zeta_2,\quad \chi_3^{22}=4\zeta_2^2\,. \end{aligned} \tag{4.17}$$

Computing the Θ_k^{ij}'s, $i,j=1,2$, $k=1,2,3$, we obtain

$$\begin{aligned} &\sum_{j=1}^{2}\Theta_1^{1j}=2\zeta_1,\quad \sum_{j=1}^{2}\Theta_2^{1j}=0,\quad \sum_{j=1}^{2}\Theta_3^{1j}=4\zeta_1\,,\\ &\sum_{j=1}^{2}\Theta_1^{2j}=0,\quad \sum_{j=1}^{2}\Theta_2^{2j}=2\zeta_2,\quad \sum_{j=1}^{2}\Theta_3^{2j}=4\zeta_2\,. \end{aligned} \tag{4.18}$$

By using (4.17) in (4.12), we get

$$\begin{aligned} a_{11} &= -(k^2/2)I_{13}\zeta_1^2\,,\\ a_{12}+a_{21} &= (k^2/2)[I_1(1+\zeta_1^2\zeta_2^2)+2I_3\zeta_1\zeta_2]\,,\\ a_{22} &= -(k^2/2)I_{13}\zeta_2^2=a_{11}^*\,, \end{aligned} \tag{4.19}$$

where we set $I_{13}\equiv I_1+I_3$. Note that the I_k's, $k=1,2,3$, are *real* [cf. (4.13)]. Similarly, by using (4.18) in (3.24), we get

$$\begin{aligned} b_1 &= -(k^2/2)(I_{13}+iI_2)\zeta_1\,,\\ b_2 &= -(k^2/2)(I_{13}-iI_2)\zeta_2=b_1^*\,. \end{aligned} \tag{4.20}$$

Similarly, as

$$\begin{aligned} &\chi_1^{13}=-\zeta_1^2\zeta_2\zeta_3,\quad \chi_1^{31}=3\zeta_1\zeta_3\,,\\ &\chi_3^{13}=4\zeta_1\zeta_3\,,\\ &\chi_1^{23}=\zeta_2\zeta_3,\quad \chi_1^{32}=-3\zeta_1\zeta_2^2\zeta_3\,,\\ &\chi_3^{23}=-4\zeta_2\zeta_3\,,\\ &\chi_1^{14}=-3\zeta_1^2\zeta_2\zeta_4,\quad \chi_1^{41}=\zeta_1\zeta_4\,,\\ &\chi_3^{14}=-4\zeta_1\zeta_4\,,\\ &\chi_1^{24}=3\zeta_2\zeta_4,\quad \chi_1^{42}=-\zeta_1\zeta_2^2\zeta_4\,,\\ &\chi_3^{24}=4\zeta_2\zeta_4\,,\\ &\chi_1^{34}=-9\zeta_1\zeta_2\zeta_3\zeta_4,\quad \chi_1^{43}=-\zeta_1\zeta_2\zeta_3\zeta_4\,,\\ &\chi_3^{34}=-4\zeta_3\zeta_4\,,\\ &\chi_1^{33}=-3\zeta_1\zeta_2\zeta_3^2,\quad \chi_3^{33}=4\zeta_3^2\,,\\ &\chi_1^{44}=-3\zeta_1\zeta_2\zeta_4^2,\quad \chi_3^{44}=4\zeta_4^2\,, \end{aligned} \tag{4.21}$$

by using (4.12) we obtain readily

$$\begin{aligned} &a_{13}+a_{31}=(k^2/2)[\zeta_1\zeta_2I_1-(3I_1+2I_3)]\zeta_1\zeta_3\equiv\alpha_{13}\zeta_3\,,\\ &a_{23}+a_{32}=(k^2/2)[3\zeta_1\zeta_2I_1+(2I_3-I_1)]\zeta_2\zeta_3\equiv\alpha_{23}\zeta_3\,,\\ &a_{14}+a_{41}=(k^2/2)[3\zeta_1\zeta_2I_1+(2I_3-I_1)]\zeta_1\zeta_4\equiv\alpha_{14}\zeta_4\,,\\ &a_{24}+a_{42}=(k^2/2)[\zeta_1\zeta_2I_1-(3I_1+2I_3)]\zeta_2\zeta_4\equiv\alpha_{24}\zeta_4\,,\\ &a_{34}+a_{43}=k^2[5\zeta_1\zeta_2I_1+I_3]\zeta_3\zeta_4\equiv\alpha_{34}\zeta_3\zeta_4\,,\\ &a_{33}=(k^2/2)[3\zeta_1\zeta_2I_1-I_3]\zeta_3^2\equiv\alpha_{33}\zeta_3^2\,,\\ &a_{44}=(k^2/2)[3\zeta_1\zeta_2I_1-I_3]\zeta_4^2\equiv\alpha_{44}\zeta_4^2\quad(\alpha_{44}\equiv\alpha_{33})\,. \end{aligned} \tag{4.22}$$

The quantities α_{ij} depend only on ζ_1 and ζ_2.

As for the b_i's we obtain

$$\begin{aligned} &\sum_{j=1}^{4}\Theta_1^{3j}=3\zeta_3(1-\zeta_1\zeta_2)\,,\\ &\sum_{j=1}^{4}\Theta_2^{3j}=-\zeta_3(3\zeta_1\zeta_2-1)\,,\\ &\sum_{j=1}^{4}\Theta_3^{3j}=4\zeta_3\,,\\ &\sum_{j=1}^{4}\Theta_1^{4j}=(1-3\zeta_1\zeta_2)\zeta_4\,,\\ &\sum_{j=1}^{4}\Theta_2^{4j}=3\zeta_4(1-\zeta_1\zeta_2)\,,\\ &\sum_{j=1}^{4}\Theta_3^{4j}=4\zeta_4\,, \end{aligned} \tag{4.23}$$

and hence,

$$\begin{aligned} b_3 &= (k^2/2)\zeta_3[3\zeta_1\zeta_2I_1-(2I_1+I_3)-iI_2]\equiv\beta_3\zeta_3\,,\\ b_4 &= (k^2/2)\zeta_4[3\zeta_1\zeta_2I_1-(2I_1+I_3)+iI_2]\\ &= b_3^*\equiv\beta_3^*\zeta_4\equiv\beta_4\zeta_4\,, \end{aligned} \tag{4.24}$$

where β_3 depends only on ζ_1,ζ_2.

Finally we need the quantities d_i, $i=1,...,4$ [cf. (3.8),

(3.29)]. Recalling (3.27) and (3.10), (3.11), we have

$$c_1 = c_2 = 0\,,$$
$$c_3 = 3i\,(k/2)\,\sigma(\zeta_1\zeta_2 + 1)\zeta_1, \tag{4.25}$$
$$c_4 = -3i\,(k/2)\,\sigma(\zeta_1\zeta_2 + 1)\zeta_2\,.$$

Then

$$d_1 = k(i\theta - \gamma)z_0, \quad d_2 = d_1^*\,, \tag{4.26}$$
$$d_3 = c_3 + \Delta c_3, \quad d_4 = d_3^*\,,$$

where

$$\Delta c_3 \equiv k_1 + k_2\zeta_3, \quad \Delta c_4 = (\Delta c_3)^*\,, \tag{4.27}$$

having set

$$k_1 \equiv -\tfrac{3}{2}k\delta(1 + \zeta_1\zeta_2)\zeta_1, \quad k_2 \equiv -k(2\gamma - i\theta)\,. \tag{4.28}$$

Now we return to (4.7). By using (4.10), (4.22), (4.24), and (4.26), it becomes

$$\begin{aligned} U_\tau = {} & \mathscr{L}[\mathscr{A}] + \mathscr{L}[\mathscr{B}]\zeta_3 + \mathscr{L}[\mathscr{C}]\zeta_4 \\ & + (\beta_3\zeta_3 + d_3)\mathscr{B} + \alpha_{13}\zeta_3\frac{\partial\mathscr{B}}{\partial\zeta_1} \\ & + \alpha_{23}\zeta_3\frac{\partial\mathscr{B}}{\partial\zeta_2} + (\beta_4\zeta_4 + d_4)\mathscr{C} \\ & + \alpha_{14}\zeta_4\frac{\partial\mathscr{C}}{\partial\zeta_1} + \alpha_{24}\zeta_4\frac{\partial\mathscr{C}}{\partial\zeta_2}, \end{aligned} \tag{4.29}$$

where the coefficients depend only on ζ_1,ζ_2.

By identifying the coefficients of ζ_3,ζ_4 and the "constant" when we compare (4.29) with $U_\tau = \mathscr{A}_\tau + \mathscr{B}_\tau\zeta_3 + \mathscr{C}_\tau\zeta_4$, we obtain the system

$$\begin{aligned} \mathscr{A}_\tau &= \mathscr{L}[\mathscr{A}] + (c_3 + k_1)\mathscr{B} + (c_4 + k_1^*)\mathscr{C}\,, \\ \mathscr{B}_\tau &= \mathscr{L}[\mathscr{B}] + \alpha_{13}\frac{\partial\mathscr{B}}{\partial\zeta_1} + \alpha_{23}\frac{\partial\mathscr{B}}{\partial\zeta_2} + (\beta_3 + k_2)\mathscr{B}\,, \\ \mathscr{C}_\tau &= \mathscr{L}[\mathscr{C}] + \alpha_{14}\frac{\partial\mathscr{C}}{\partial\zeta_1} + \alpha_{24}\frac{\partial\mathscr{C}}{\partial\zeta_2} + (\beta_4 + k_2^*)\mathscr{C}\,, \end{aligned} \tag{4.30}$$

to which we associate the *initial values* (4.6).

Remark 4.1: If $E\{n(\cdot)\} \in L[0,\infty)$ and $\delta = \gamma = \theta = 0$, we have $d_i(\zeta) \equiv 0$ for every i (cf. Sec. III). In this case $\mathscr{A}$ is *uncoupled from* $\mathscr{B}$, $\mathscr{C}$ and therefore the effects due to nonlinearity are negligible. However, the stationarity of $n(\cdot)$ would imply $E\{n(\cdot)\} \equiv \sigma \equiv 0$, in this case.

Remark 4.1': The equations for $\mathscr{B}$, $\mathscr{C}$ are always *uncoupled* from each other and from the equation satisfied by $\mathscr{A}$. It is clear from this and from the IV's (4.6) that $\mathscr{B} = \mathscr{C}^*$, as $\zeta_2 = \zeta_1^*$.

Therefore we can confine ourselves to the system for $\mathscr{A}$ and $\mathscr{C}$ *only*:

$$\begin{aligned} \mathscr{A}_\tau &= \mathscr{L}[\mathscr{A}] + (c_4 + k_1^*)^*\mathscr{C} + (c_4 + k_1^*)^*\mathscr{C}^*\,, \\ \mathscr{C}_\tau &= \mathscr{L}[\mathscr{C}] + \alpha_{14}\frac{\partial\mathscr{C}}{\partial\zeta_1} + \alpha_{24}\frac{\partial\mathscr{C}}{\partial\zeta_2} + (\beta_4 + k_2^*)\mathscr{C}\,, \end{aligned} \tag{4.31}$$

with

$$\mathscr{A}(\zeta_1,\zeta_2;0) = \zeta_1,\zeta_2, \quad \mathscr{C}(\zeta_1,\zeta_2;0) = w\zeta_1\,. \tag{4.32}$$

By solving such a system, we shall obtain $E\{|R_0|^2\} + 2w\,\mathrm{Re}\,E\{R_0 R_1^*\} = U(0,0,0,0;\tau) = \mathscr{A}(0,0;\tau)$.

Let us introduce *polar coordinates* ρ,ϕ, being $\zeta_1 = \rho e^{i\phi}$, $\zeta_2 = \rho e^{-i\phi}$, and set

$$\begin{aligned} \mathscr{A}(\zeta_1,\zeta_2;\tau) &\equiv a(\rho,\tau)\,, \\ \mathscr{C}(\zeta_1,\zeta_2;\tau) &\equiv w\,c(\rho,\tau)e^{i\phi}\,. \end{aligned} \tag{4.33}$$

This amounts to performing a Fourier analysis on the system above. It is clear from the IV's (4.32) that only the phase-independent component of $\mathscr{A}(\rho e^{i\phi}, \rho e^{-i\phi};\tau)$ is nonzero, etc. We get

$$\begin{aligned} \frac{\partial c}{\partial\tau_1} &= (1-\rho^2)^2\frac{\partial^2 c}{\partial\rho^2} + \left[\frac{(1-\rho^2)(1-9\rho^2)}{\rho} - \chi_1\rho\right]\frac{\partial c}{\partial\rho} \\ &\quad + \left[-\frac{(1+\rho^2)^2}{\rho^2} + 4(4\rho^2 - 1) - 2\chi_1\right]c\,, \\ &\quad 0<\rho<1, \quad \tau_1>0\,, \\ \frac{\partial a}{\partial\tau_1} &= (1-\rho^2)^2\frac{\partial^2 a}{\partial\rho^2} + \left[\frac{(1-\rho^2)^2}{\rho} - \chi_1\rho\right]\frac{\partial a}{\partial\rho} \\ &\quad + \frac{12}{kI_1}(1+\rho^2)\,\rho\,w[(i\sigma+\delta)c - (i\sigma-\delta)c^*]\,, \\ &\quad 0<\rho<1, \quad \tau_1>0\,, \\ c(\rho,0) &= \rho, \quad 0<\rho<1\,, \\ a(\rho,0) &= \rho^2, \quad 0<\rho<1\,, \end{aligned} \tag{4.34}$$

where

$$\tau_1 \equiv (k^2/8)I_1\tau \quad (\tau \equiv \epsilon^2 L)\,, \tag{4.35}$$

$$\chi_1 \equiv 8\gamma/kI_1\,. \tag{4.36}$$

Observe that the equation for c as well as its IV is *real*. Therefore $c^* = c$ and, in the equation for a, the coupling term becomes

$$-(24\delta/kI_1)w(1+\rho^2)\,\rho\,c\,. \tag{4.37}$$

Moreover, we can "remove" the singular term $\sim -(1/\rho^2)c$ in the equation for c, by setting

$$c \equiv \hat{c}/\rho\,. \tag{4.38}$$

The easy calculations yield

$$\begin{aligned} \frac{\partial\hat{c}}{\partial\tau_1} &= (1-\rho^2)^2\frac{\partial^2\hat{c}}{\partial\rho^2} - \left[\frac{(1-\rho^2)(1+7\rho^2)}{\rho} + \chi_1\rho\right]\frac{\partial\hat{c}}{\partial\rho} \\ &\quad - (\chi_1 - 8\rho^2)\hat{c}, \quad 0<\rho<1, \quad \tau_1>0\,, \\ \frac{\partial a}{\partial\tau_1} &= (1-\rho^2)^2\frac{\partial^2 a}{\partial\rho^2} \\ &\quad + \left[\frac{(1-\rho^2)^2}{\rho} - \chi_1\rho\right]\frac{\partial a}{\partial\rho} - w\chi_2(1+\rho^2)\hat{c}\,, \\ &\quad 0<\rho<1, \quad \tau_1>0\,, \\ \hat{c}(\rho,0) &= \rho^2, \quad 0<\rho<1\,, \\ a(\rho,0) &= \rho^2, \quad 0<\rho<1\,, \end{aligned} \tag{4.39}$$

where we set

$$\chi_2 \equiv 24\delta/kI_1\,. \tag{4.40}$$

The *loss parameters* χ_1,χ_2 ($\chi_1>0, \chi_2>0$) are, essentially, *damping-to-noise ratios*. System (4.39) is a *weakly cou-*

pled parabolic system, linear though *degenerate* at $\rho = 1$ and *singular* at $\rho = 0$. The parameter χ_2 is responsible for the coupling between the two equations in (4.39): if $\chi_2 = 0$ no effect due to the nonlinearity can be observed in our model. It can also magnify the effect of a small $w > 0$.

Several consequences of our analysis can be drawn at this point. First of all we can recover the *linear lossless* as well as the *linear lossy* problem, as special cases.

A. The linear problem

Using polar coordinates, the operator $\mathscr{L}$ in (3.32) becomes

$$\mathscr{L}_{\rho,\phi} \equiv \frac{k^2}{8} I_1 \left\{ (1-\rho^2)^2 \frac{\partial^2}{\partial \rho^2} + \left[\frac{(1-\rho^2)^2}{\rho} - \chi_1 \rho \frac{\partial}{\partial \rho} \right] + [(1+\rho^2)^2 + 4r_{31}\rho^2] \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} + (\chi_0 - 4r_{21}) \frac{\partial}{\partial \phi} \right\}, \tag{4.41}$$

where we set $r_{21} \equiv I_2/I_1$, $\chi_0 \equiv 8\theta/kI_1$.

As the coefficients in (4.41) are independent of ϕ, we can restrict ourselves to the marginal generator, involving ρ only:

$$\mathscr{L}_\rho \equiv \frac{k^2}{8} I_1 \left\{ (1-\rho^2)^2 \frac{\partial^2}{\partial \rho^2} + \left[\frac{(1-\rho^2)^2}{\rho} - \chi_1 \rho \right] \frac{\partial}{\partial \rho} \right\}. \tag{4.42}$$

Then we are able to compute the transition probability density $P(\rho, L)$ for the process $\rho(L)$, given $\rho(0) = 0$, by integrating the appropriate *forward* equation (recall that $\rho = |\zeta_1| \equiv |z_0| \equiv |R_0|$). Then $E\{|R_0|^2\}$ is computed by integrating with respect to such a measure P. Explicit formulas can be obtained in this case, both for P and $E\{|R_0|^2\}$ for the *lossless* problem, $\chi_1 = 0$ (cf. Ref. 6). The *lossy* problem and the stationary distribution existing in such a case have been studied in Ref. 12.

Alternatively, $E\{|R_0|^2\}$ can be evaluated directly by solving the *backward* equation, as follows. Setting $\mathscr{L}_\rho \equiv (k^2/8) I_1 \mathscr{L}'_\rho$ in (4.42), consider the problem

$$\begin{aligned} &u_{\tau_1} = \mathscr{L}'_\rho [u], \quad 0 < \rho < 1, \quad \tau_1 > 0, \\ &u(\rho, 0) = \rho^2, \quad 0 < \rho < 1. \end{aligned} \tag{4.43}$$

The linear parabolic equation in (4.42) is *singular* at the end point $\rho = 0$ and *degenerate* at $\rho = 1$. As both, the equation and the IV in (4.43), are *symmetric* in ρ, we can assume

$$u_\rho(0, \tau_1) = 0, \tag{4.44}$$

which permits us to dominate the singularity at $\rho = 0$. *No* boundary condition is needed on $\rho = 1$.

Finally, we obtain [recalling (4.35)]

$$\begin{aligned} E\{|R_0|^2\}(\tau_1) &= u(0, \tau_1)|_{\tau_1 = (k^2/8) I_1 \epsilon^2 L} \\ &= u(0, (k^2/8) I_1 \epsilon^2 L). \end{aligned} \tag{4.45}$$

The graph of $E\{|T_0|^2\} = 1 - E\{|R_0|^2\}$ for $\chi_1 = 0$ is plotted in Ref. 6, p. 17 (see also Ref. 5).

Let us go back to the general case.

B. The nonlinear lossless problem

It is rather surprising to discover that the model we have been studying does *not* exhibit *any* new effect when the nonlinearity acts jointly with the randomness and dissipation is neglected. This is evident from system (4.39): In fact, if we set $\delta = 0$, the two equations *decouple* as when we set $w = 0$, and then $a(0, \tau_1)$ yields the quantity $E\{|R_0|^2\}$ of the *linear* case.

Our goal is to compute the first *nontrivial* correction to $E\{|R_0|^2\}$, due to nonlinearity. As there is no contribution from terms of the order $O(w)$, we went further and computed the correction of order $O(w^2)$. This can be done by generalizing, in a rather obvious way, the method we followed to compute the $O(w)$ correction. The rather elementary calculations are, however, lengthy and very cumbersome. We do not give here any details but just the conclusion: The surprising result is that *also* the $O(w^2)$ correction vanishes. We state this result as a theorem.

Theorem 4.2: The mean power reflected from a slab $[0, L]$ of a one-dimensional nonlinear lossless random medium, described by the refractive index given by (2.1), (2.4) with $\delta = \gamma = 0$, is unaffected by the nonlinearity whose intensity is w, at least up to the order $O(w^2)$, in the diffusion limit $\epsilon \to 0$, $L \to \infty$, with $\epsilon^2 L = \text{const}$.

The same conclusion holds true even changing w into $-w$, though this represents a quite different physical problem.

We stress the fact that the *scaling* assumptions in (2.4) play a decisive role in such a result.

Also note that the values $\sigma \equiv E\{n(x)\}$ and $\theta \equiv E\{\theta(x)\}$ do *not* play any role. Indeed, we can see from the conservation of the energy associated with Eq. (2.1) that only the imaginary part of the index of refraction matters. Let us write (2.1), for short, in the form

$$v'' + f(x) v = 0, \tag{4.46}$$

with $v(x) \equiv u^\epsilon, f(x) \equiv k^2(1 + \tilde{\epsilon})$, and $\tilde{\epsilon}$ defined in (2.4). By multiplying the left-hand side of (4.46) by v^*, and the equation obtained from (4.46) by taking the complex conjugate, by v, and subtracting side by side, we get

$$(v'v^* - v^{*\prime} v)' + 2i \operatorname{Im} f(x) |v|^2 = 0. \tag{4.47}$$

This can be integrated between 0 and L, yielding

$$\begin{aligned} &(v'v^* - v^{*\prime} v)(L) \\ &\quad = (v'v^* - v^{*\prime} v)(0) - 2i \int_0^L \operatorname{Im} f(\xi) |v(\xi)|^2 d\xi, \end{aligned} \tag{4.48}$$

and using the BV's (2.6) and (2.7), we obtain

$$|T|^2 = 1 - |R|^2 - \int_0^L \frac{1}{k} \operatorname{Im} f(\xi) |v(\xi)|^2 d\xi. \tag{4.49}$$

From (2.4) we get

$$P_T + P_R + P_D = 1, \tag{4.50}$$

where we set

$$\begin{aligned} &P_T \equiv |T|^2, \quad P_R \equiv |R|^2, \\ &P_D \equiv k\epsilon^2 \int_0^L (\delta w |u^\epsilon(\xi, L, w)|^2 + \gamma) |u^\epsilon(\xi, L, w)|^2 d\xi. \end{aligned} \tag{4.51}$$

Here P_T, P_R, P_D are, respectively, the transmitted, reflected, and dissipated powers. Note that P_D depends on *all values* of

the field inside the slab $[0,L]$, and this still holds true in the linear lossy problem ($w=0$, but $\gamma>0$).

From (4.51) follows, of course,

$$0<P_T<1, \quad 0<P_R<1, \quad 0<P_D<1. \tag{4.52}$$

It is clear that we cannot compute P_T from (4.50), knowing only P_R, which is possible, on the other hand, in the lossless problem ($P_D\equiv 0$). The same relations (4.50) and (4.52) hold, replacing P_T, P_R, P_D with their expected values.

C. The nonlinear lossy problem

Let us go back finally to the full problem (2.13), described statistically, in the diffusion limit, by the system (4.39), with $\chi_1>0$, $\chi_2>0$, $w>0$. Its solution will enable us to compute the $O(w)$ correction to $E\{|R_0|^2\}$ due to nonlinearity, in the lossy case. In the next section we shall perform a numerical integration of the system (4.39), for several values of χ_1, χ_2, w. Some information, however, can be obtained at once from (4.39), by direct inspection.

It is easy to check that the same system (4.39) with the IV $a(\rho,0)=0$ instead of $a(\rho,0)=\rho^2$ yields $a(0,\tau_1)=\operatorname{Re} E\{R_0 R_1^*\}$, i.e., the correction term alone (the coefficient of $2w$, to be more precise). In fact, this corresponds to setting $U|_{\tau=0}=\zeta_1\zeta_4$ in (4.3). From this it is clear that the solution $\hat{c}$ will be positive and thus $a<0$ (as $\chi_2>0$). Therefore

$$E\{|R_0|^2\}+2w \operatorname{Re} E\{R_0 R_1^*\}<E\{|R_0|^2\}, \tag{4.53}$$

for $w>0$, i.e., the mean reflected power is *smaller* due to the nonlinearity, with respect to the linear (dissipative) case. However, this does *not* mean at all that the mean transmitted power is greater, since in the dissipative case the relation $P_T+P_R=1$ is replaced by (4.50).

V. NUMERICAL TREATMENT

In this section we shall describe the numerical treatment that we performed on the parabolic system (4.39). Our primary goal is to compute $a(0,\tau_1)$ because

$$E\{|R|^2\}\cong E\{|R_0|^2\}+2w \operatorname{Re} E\{R_0 R_1^*\}=a(0,\tau_1)$$

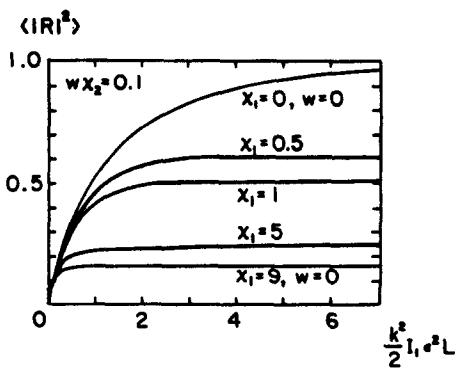

FIG. 1. Mean reflected power versus $(k^2/2)I_1\epsilon^2 L$ for different values of the loss parameter χ_1 ($\chi_1=0.5, 1, 5, 9$) and $w\chi_2=0.1$ fixed.

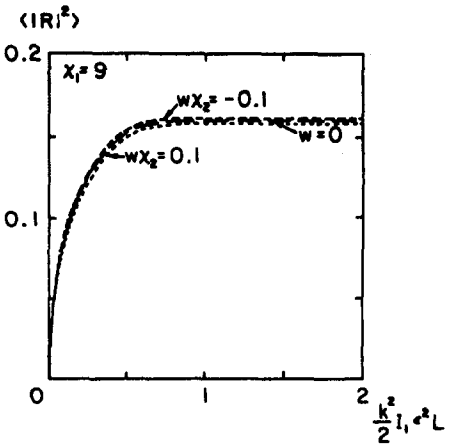

FIG. 2. Mean reflected power versus $(k^2/2)I_1\epsilon^2 L$ for $\chi_1=9$ fixed and $w\chi_2=-0.1, 0, 0.1$.

[cf. (4.4), (4.5), (4.33)]. The problem is nontrivial because of the singularities at $\rho=0, \rho=1$, and must be completed by specifying *whether* suitable boundary conditions are needed on $\rho=0$ and $\rho=1$ *and*, in case the answer should be affirmative, *which* boundary conditions they are.

As for the boundary $\rho=0$, we can exploit the fact that both, the equations and the IV's in (4.39), are symmetric in ρ, around $\rho=0$. It follows that the solution of (4.39) satisfies the conditions

$$\left.\frac{\partial \hat{c}}{\partial \rho}\right|_{\rho=0}=\left.\frac{\partial a}{\partial \rho}\right|_{\rho=0}=0 \tag{5.1}$$

[cf. (4.44)].

We observe that

$$\left.\frac{\partial \hat{c}}{\partial \rho}\right|_{\rho=0}=\left.\left[\rho\frac{\partial c}{\partial \rho}+c\right]\right|_{\rho=0}=c(0^+,\tau_1) \tag{5.2}$$

(as long as $\rho\,\partial c/\partial\rho\to 0$ as $\rho\to 0^+$, e.g., if $\partial c/\partial\rho$ is *bounded* up to $\rho=0$). Equation (5.3) tells us that $\partial\hat{c}/\partial\rho$ is "well behaved" as $\rho\to 0^+$. However, we do *not* know $c(0^+,\tau_1)$ and we shall use the boundary condition $(\partial\hat{c}/\partial\rho)|_{\rho=0}=0$, by symmetry.

Conditions (5.1) allow us to dominate the *singularity* at $\rho=0$, as they enable us to replace the terms like $[(\beta(\rho)/\rho)\hat{c}_\rho]|_{\rho=0}$ by $\beta(0)\hat{c}_{\rho\rho}|_{\rho=0}$, in the numerical scheme.

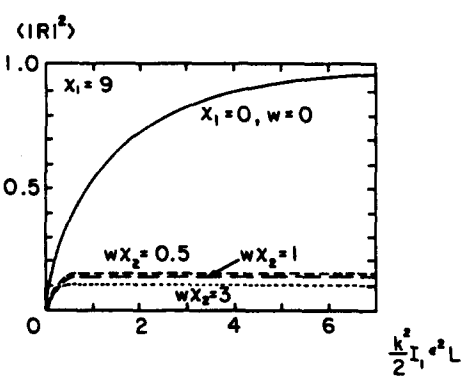

FIG. 3. Mean reflected power versus $(k^2/2)I_1\epsilon^2 L$ for $\chi_1=9$ fixed and $w\chi_2=0.5, 1, 3$.

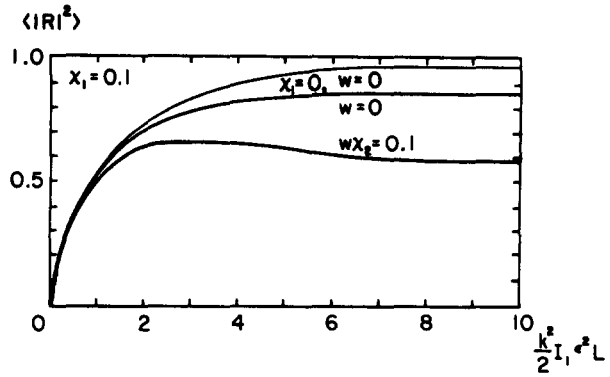

FIG. 4. Mean reflected power versus $(k^2/2)I_1\epsilon^2 L$ for $\chi_1 = 0.1$, $w\chi_2 = 0.1$ compared with the corresponding linear lossy case ($\chi_1 = 0.1$, $w = 0$).

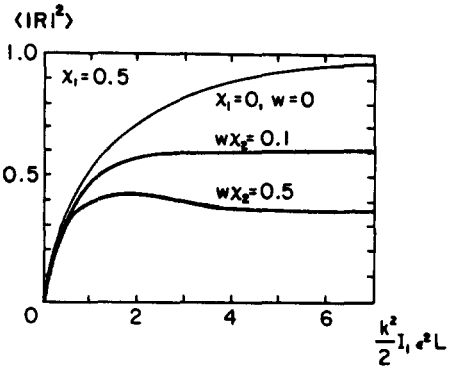

FIG. 6. Mean reflected power versus $(k^2/2)I_1\epsilon^2 L$ for $\chi_1 = 0.5$ fixed and $w\chi_2 = 0.1, 0.5, 1$. Also the case $\chi_1 = 0.5$, $w\chi_2 = 0.1$ is plotted.

As for the boundary $\rho = 1$, if we consider the "limiting" form of the system (4.39) for $\rho \approx 1$, we obtain the *hyperbolic system* (nonstrictly hyperbolic *at* $\rho = 1$)

$$\frac{\partial \hat{c}}{\partial \tau_1} = -[\chi_1 + (16-\chi_1)(1-\rho)]\frac{\partial \hat{c}}{\partial \rho} - [\chi_1 - 8 + 16(1-\rho)]\hat{c}\,,$$

$$\frac{\partial a}{\partial \tau_1} = -\chi_1 \rho \frac{\partial a}{\partial \rho} - 2\chi_2 \rho\, \hat{c}\,, \tag{5.3}$$

with the IV's

$$\hat{c}(\rho,0) = \rho^2 \approx 1, \quad a(\rho,0) = \rho^2 \approx 1\,. \tag{5.4}$$

We shall use (5.3) *on* the boundary $\rho = 1$ and in this way we handle the *degeneracy* of (4.39) at $\rho = 1$. In the *linear* problem, (5.3) reduces to the equation for a with $w = 0$.

Note that, under the hypothesis $\chi_1 > 0$ (dissipation), (5.3) is a hyperbolic system with *outgoing flow*. Therefore, no boundary condition is needed at $\rho = 1$, as is known.

The actual implementation of system (4.39) has been done by using an *implicit scheme of finite differences*, namely forward time differences and space-centered differences (the Cranck–Nicholson scheme). At $\rho = 0$, the Neumann conditions (5.1) were used, while at $\rho = 1$ we solved the problem [(5.3), (5.4)] as follows. We used, essentially, a Cranck–Nicholson scheme *at the point* $(N - \frac{1}{2}, j + \frac{1}{2}), N + 1$ corresponding to the location $\rho = 1$ (and thus $N - \frac{1}{2}$ to $1 - \Delta\rho/2$), and j being the time index, in order to retain *second-order* accuracy.

In Fig. 1 we plotted

$$a(0,\tau_1) \equiv E\{|R_0|^2\} + 2w\,\mathrm{Re}\,E\{R_0 R_1^*\} \cong E\{|R|^2\}\,,$$

as a function of $(k^2/2)I_1\epsilon^2 L \propto \tau_1$, for $w\chi_2 = 0.1$ and various values of χ_1 ($\chi_1 = 0.5,1,5,9$). In this figure as well as in all the others, the upper curve approaching 1 when $\tau_1 \to \infty$ represents $E\{|R_0|^2\}$, obtained in the linear lossless case $w = 0$, $\chi_1 = 0$ (cf. Ref. 6).

When χ_1 is increased, the corresponding curves are lowered: In fact, we expect that the mean transmitted power decay to zero, by some localization property, and thus the mean dissipated power increase with χ_1. Note that χ_1 also affects the linear problem alone.

In Fig. 2, we compare the graphs of $a(0,\tau_1)$ corresponding to $\chi_1 = 9$ and $w\chi_2 = -0.1, 0$, and 0.1. In Fig. 3 we kept fixed $\chi_1 = 9$ and varied $w\chi_2$ ($w\chi_2 = 0.5,1,3$). Again, increasing $w\chi_2$ shows an increased dissipation. Note that, while w must be chosen "small" if we want $a(0,\tau_1)$ to approximate $E\{|R|^2\}$ [cf. (2.12)], a large χ_2 can *magnify* its effect, because w enters the system (4.39) only via the *product* $w\chi_2$. Anyway, it is the parameter $w\chi_2 \neq 0$ that allows the coupling between the two equations in system (4.39): If $\chi_2 = 0$, there is no effect due to nonlinearity, in this model, as when $w = 0$, even though $\chi_1 > 0$.

In Fig. 4 the graph of $a(0,\tau_1)$, obtained for $\chi_1 = 0.1$ and

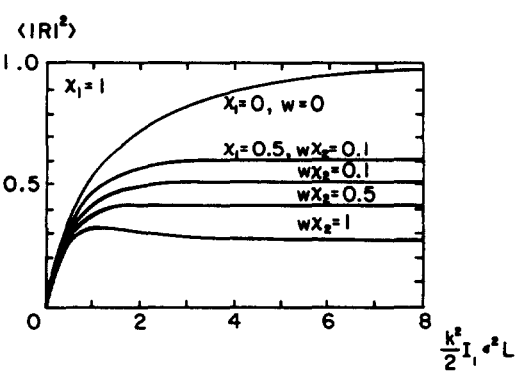

FIG. 5. Mean reflected power versus $(k^2/2)I_1\epsilon^2 L$ for $\chi_1 = 1$ fixed and $w\chi_2 = 0.1, 0.5, 1$.

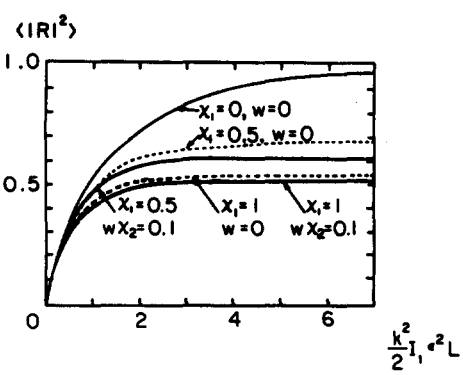

FIG. 7. Mean reflected power versus $(k^2/2)I_1\epsilon^2 L$ for $\chi_1 = 0.5$ [$\chi_1 = 1$] and $w = 0$ (linear case), and $\chi_1 = 0.5$ [$\chi_1 = 1$] and $w\chi_2 = 0.1$.

$w\chi_2 = 0.1$ is compared with the corresponding linear lossy case ($\chi_1 = 0.1$, $w = 0$). In Fig. 5 we show several graphs of $a(0,\tau_1)$, obtained for the fixed value of $\chi_1 = 1$, by varying $w\chi_2$ ($w\chi_2 = 0.1, 0.5, 1$). The same is done in Fig. 6, for $\chi_1 = 0.5$. In Fig. 5, however, the curve corresponding to $\chi_1 = 0.5$ and $w\chi_2 = 0.1$ is also drawn, for comparison.

In Fig. 7, finally, we show, for the purpose of comparison, the graphs obtained in the *linear* case $w = 0$, $\chi_1 = 0.5$, *and* the *nonlinear* case $w\chi_2 = 0.1$, $\chi_1 = 0.5$, as well as the like when $\chi_1 = 1$.

In all figures there is clear numerical evidence that some nontrivial *stationary value* exists [corresponding to the solution to system (4.39) with $\partial/\partial\tau_1 \equiv 0$]. The physical interpretation of this fact can be given as follows. The unit amplitude wave impinging on the slab of random medium penetrates and undergoes several (multiple) reflections by the random scatterers. During such a process, it is partially absorbed by the medium. The fraction that penetrates more and more deeply is completely absorbed before returning back to the interface vacuum–random medium. Therefore, if, for random fluctuations of a given size and spectral density, the slab is sufficiently thick (i.e., τ_1 is large enough), there is a *constant* amount of mean reflected power, say $P_R(\infty)$, and the same is true for the mean dissipated power, $P_D(\infty) = 1 - P_R(\infty)$ [$P_T(\infty) = 0$].

VI. CONCLUSIONS

In closing, let us summarize the results of the paper. The fact that there is *no* correction to the mean reflected power due to the nonlinearity, at least up to order $O(w^2)$, with respect to the *linear* case $w = 0$, in the *lossless* model, is rather surprising. The explanation must be sought in certain averaging operated by the nonlinear term in equation (2.1), in view of the particular scaling assumptions that assign a certain relative importance to the nonlinearity compared to the randomness. Indeed, a similar behavior has been recently observed in Ref. 17, where, essentially, the same equation (2.1) was studied, associated, however, with an *initial-value* problem. Anyway, the results obtained in this paper favorably agree with those observed in numerically simulated experiments,[18] where the case $\epsilon = O(1)$ was investigated also.

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Formulation of the inverse problem for the reduced wave equation in momentum space

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The direct and inverse problem associated with the reduced wave equation expressed in momentum space (Fourier transform space of the spatial variable) is considered. It is shown that the right inverse of the scattering operator associated with complex scattered field amplitude $T(k',k)$ exists for the case where the index of refraction $n(x)$ is real and satisfies certain smoothness conditions. A quadratic integral equation involving only $T(k',k)$ is obtained that represents a necessary and sufficient condition for $T(k',k)$ to be a complex scattered field amplitude associated with a real index of refraction. For the actual physical inverse problem where only on-shell ($|k'| = |k|$) values of $T(k',k)$ are known, the inverse problem involves solving this nonlinear system for off-shell data from on-shell data. Several other nonlinear systems that can be used are derived. Once $T(k',k)$ is known for k',k, $n(x)$ is readily obtained.

I. INTRODUCTION

The direct and inverse scattering problem associated with the reduced wave equation expressed in momentum space (the Fourier transform space of the spatial variable) is considered. The advantage of this approach is that the direct and inverse problems are related through a single integral equation. Such an approach has been extensively treated in the literature for the Schrödinger equation (see Faddeev,[1] Newton,[2] and Friedrichs[3]). The advantage that the Schrödinger equation has over the wave equation is that the potential can be treated as a perturbation of an operator, and the inverse problem then involves the perturbation of the spectrum. Such is not the case for the wave equation. There have been attempts[4–6] to treat the reduced wave equation in momentum space, but the emphasis has been on obtaining a Born or Neumann-type series solution to the problem.

A key assumption that will be taken throughout is that the index of refraction $n(x)$ will be real.

In Sec. II, the direct scattering problem is formulated in the Fourier transform space of the spatial variable $x \in \mathbf{R}^3$. The well-known integral equation [Eq. (8)] in momentum space relating the inverse transform $V(k)$ of $n^2(x) - 1$ and the far scattered field complex amplitude $T(k',k)$ is given. In Sec. III, asymptotic estimates and smoothness properties on these latter two quantities are derived.

In Sec. IV, a necessary condition is formulated to insure that $T(k',k)$ be a solution of the integral equation [Eq. (8)] corresponding to real index of refraction. This condition [Eq. (17) of Lemma 1] is a quadratic nonlinear integral equation involving $T(k',k)$ only.

It is shown in Sec. V that the reality condition on $n(x)$ implies the existence of a right inverse of an operator, which is the sum of the identity and a singular integral operator containing $T(k',k)$ in its kernel. Conditions for which the operator is unitary are given.

In Secs. VI and VIII, this operator is used to show that the inversion of Eq. (8) leads to a solution corresponding to a real index of refraction. [By inversion, we mean, given $T(k',k)$ for all $k',k \in \mathbf{R}^3$, to determine $V(k)$ uniquely.]

Finally, in Sec. VIII, the inverse scattering problem is formulated. It involves solving the nonlinear integral equation (17) to obtain values of $T(k',k)$ for all $k',k \in \mathbf{R}^3$ from knowledge of on-shell values $|k'| = |k|$ only. Other nonlinear systems useful for determining off-shell values from on-shell values are presented. Once $T(k',k)$ is known for all $k',k \in \mathbf{R}^3$, then $n(x)$ can be recovered.

In the analysis that follows, the following notation will be used: If $k \in \mathbf{R}^3$, then $k^2 = k \cdot k$ and $|k| = (k \cdot k)^{1/2}$.

In addition we will define the Hilbert space $\mathscr{H}$ of $\mathscr{L}_2(\mathbf{R}^3)$ functions with inner product

$$(f,g) = \int_{\mathbf{R}^3} f(p)\bar{g}(p)dp,$$

as well as the Hilbert space $\mathscr{H} \otimes \mathscr{H}$ of functions $g(k',k)$ of the two variables $k,k' \in \mathbf{R}^3$. Here the inner product is given by

$$(f,g) = \iint_{\mathbf{R}^3 \times \mathbf{R}^3} f(p,q)\bar{g}(p,q)dp\,dq.$$

II. DIRECT SCATTERING PROBLEM

From Leis[7] the scattering problem associated with an incident plane wave $u^i(x,k) = \exp(ik \cdot x)$,

$$\Delta u^s + k^2 n^2(x) u^s = -k^2(n^2(x) - 1)u^i, \quad x \in \mathbf{R}^3,$$

$$\lim_{r \to \infty} \left(\frac{\partial u^s}{\partial r} - iku^s \right) \to 0, \quad r = |x|, \tag{1}$$

has a unique solution if $(n^2 - 1)$ is continuous and has compact support, i.e., $(n^2(x) - 1) \in C_0(\mathbf{R}^3)$. Here of course $u^s(x,k)$ represents the scattered field.

From the integral formulation of (1),

$$u(x,k) = u^i(x,k) + \frac{k^2}{4\pi} \int_D [n^2(y) - 1] \times \frac{e^{i|k||x-y|}}{|x-y|} u(y,k)dy, \tag{2}$$

involving the total field $u = u^i + u^s$ [with the support of $n^2(x) - 1$ being given by the domain D], the far scattered

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field is obtained in the usual manner:

$$\lim_{|x|\to\infty} 4\pi|x|e^{-i|k||x|}u^s(x,k)\to(2\pi)^3k^2T(k',k), \quad (3)$$

where $k'=x/|x|$, and

$$T(k',k)=\frac{1}{(2\pi)^3}\int_D (n^2(y)-1)e^{-ik'\cdot y}u(y,k)dy. \quad (4)$$

The direct scattering problem is expressed in momentum space by taking the appropriate (inverse) Fourier transform. The transform pairs for the scattered field are given by

$$u^s(p,k)=\mathscr{F}^{-1}[u^s]=\frac{1}{(2\pi)^3}\int e^{-ip\cdot x}u^s(x,k)dx, \quad (5a)$$

$$u^s(x,k)=\mathscr{F}[u^s]=\int e^{ip\cdot x}u^s(p,k)dp. \quad (5b)$$

The (inverse) Fourier transform of $(n^2(x)-1)$ will be denoted by $V(p)$ as follows:

$$V(p)=\mathscr{F}^{-1}[n^2-1]$$

$$=\frac{1}{(2\pi)^3}\int_D e^{-ip\cdot x}[n^2(x)-1]dx. \quad (6)$$

By taking the (inverse) Fourier transform of Eq. (2), one obtains the well-known result[6]

$$u^s(p,k)=k^2T(p,k)/(p^2-k^2-i0), \quad (7)$$

which relates the transform of the scattered field to the far-scattered complex field amplitude. Furthermore, on replacing the total field $u(x,k)$ in Eq. (4) by

$$u(x,k)=e^{ik\cdot x}+\int e^{ip\cdot x}\frac{k^2T(p,k)dp}{p^2-k^2-i0},$$

the following equation in momentum space is obtained[6]:

$$T(k',k)=V(k'-k)+k^2\int\frac{V(k'-p)T(p,k)dp}{p^2-k^2-i0}. \quad (8)$$

The importance of this equation is that it relates the scattered far field amplitude $T(p,k)$ to the $V(k)$, the (inverse) Fourier transform of $n^2(x)-1$, and hence is useful for the direct problem (to determine T from V) and for the inverse problem (to determine V from T).

III. ESTIMATES FOR $V(k'-k)$ AND $T(k',k)$

For the direct scattering problem to be unique, $n^2(x)-1$ was required to be continuous with compact support.[7] However, it was pointed out[8] that the condition of continuity could be relaxed to allow the important physical case of piecewise continuity on $n(x)$. By this, it is meant that the domain D (the support of n^2-1) is decomposed into a finite number M of domains D_j, bounded by surfaces S_j sufficiently smooth so that Green's theorem could be employed in each region D_j. Furthermore $n(x)$ would be continuous in each region D_j with finite jump discontinuities across S_j, and both u and the normal derivative $\partial u/\partial n$ would be continuous across S_j.

From the result that $V(k)=\mathscr{F}^{-1}(n^2-1)$ and that n^2-1 is continuous or piecewise continuous with compact support, we can state that $V(k)\in C^\infty(\mathbf{R}^3)\cap\mathscr{L}_2(\mathbf{R}^3)$. Furthermore, if we define the mth partial derivative

$$\mathscr{D}^m=\frac{\partial^m}{\partial k_1^{m_1}\partial k_2^{m_2}\partial k_3^{m_3}},\quad m=m_1+m_2+m_3,\quad k_i\in\mathbf{R},$$

and m_1,m_2,m_3 are positive integers or zero, then it can be shown that

$$\mathscr{D}^mV(k)\in\mathscr{L}_2(\mathbf{R}^3),\quad \text{for all finite } m.$$

However, we cannot make any statements on the behavior of V as $|k|\to\infty$, unless we specify some smoothness. If n^2-1 is piecewise C^2 in D, then using Green's theorem in each of the subdomains D_j, it can be shown that

$$(2\pi)^3V(k)=-\frac{1}{k^2}\int_D e^{-ik\cdot x}\nabla^2n\,dx$$
$$-\frac{1}{k^2}\sum_{j=1}^m\int_{S_j}\left\{\frac{\partial e^{-ik\cdot x}}{\partial n}[n^2-1]^{\pm}\right.$$
$$\left.-e^{ik\cdot x}\left[\frac{\partial(n^2-1)}{\partial n}\right]_-^+\right\}d\sigma, \quad (9)$$

where $[n^2-1]^{\pm}$ represents the jump in value across S_j. The first term on the right-hand side of Eq. (9) is $o(1/k^2)$. The second term is zero if $n(x)$ is continuous everywhere. Otherwise it can take on values $O(1/|k|)$ to $O(1/k^2)$ depending upon whether the stationary values of integrand (points for which k is perpendicular to the surfaces) occurs at isolated convex points of finite curvature or infinite curvature, or are portions of a flat surface. The third term vanishes, of course, if $n(x)$ is C^1, otherwise this term at worst is $O(1/k^2)$.

If $n(x)$ is piecewise C^1, then it can be shown that

$$(2\pi)^3V(k)=\frac{i}{k^2}\int_D e^{-ik\cdot x}k\cdot\nabla n^2\,dx$$
$$+\frac{i}{k^2}\sum_{j=1}^m\int_{S_j}k\cdot\hat{n}_je^{-ik\cdot x}[n^2(x)-1]^{\pm}\,d\sigma,$$

where $\hat{n}_j$ is the unit normal to S_j. The first term on the right-hand side is $o(1/k^2)$ and the remaining term vanishes if $n^2(x)$ is continuous, otherwise it takes on values $O(1/|k|)$ to $O(1/k^2)$.

Henceforth, the degree of smoothness will be postulated by specifying that $V(k)$ behaves like $|k|^{-1-\theta_0}$, $0<\theta_0<1$, as $|k|\to\infty$. Since $V(k)$ is continuous and differentiable, we have the Hölder conditions

$$V(k)<C(1+|k|)^{-1-\theta_0},$$
$$|V(k+h)-V(k)|<C(1+|k|)^{-1-\theta_0}|h|^\mu,\quad |h|<1, \quad (10)$$

where the Hölder index $\frac{1}{2}<\mu<1$. The lower limit on the index μ is taken to be $\frac{1}{2}$ rather than the usual 0 because of additional restraints that will be placed later on in the analysis.

Definition: $\mathscr{S}_{\theta_0,\mu}$ is the set of Hölder-continuous functions $f(k',k)$ of the two variables k',k in $\mathbf{R}^3$ with estimating functions $(1+|k'-k|)^{-1-\theta_0}$ and indices μ, satisfying the conditions (with $|h|<1$ and $|h'|<1$)

$$|f(k',k)|<C(1+|k'-k|)^{-1-\theta_0},$$
$$|f(k'+h',k+h)-f(k',k)| \quad (11)$$
$$<C(1+|k'-k|)^{-1-\theta_0}(|h'|^\mu+|h|^\mu),$$

where $\frac{1}{2}<\mu<1$ and $0<\theta_0<1$.

Thus as a function of the two variables, $V(k'-k)$ belongs to the set $\mathscr{S}_{\theta_0,\mu}$. In addition, because $V(k)$ is continuous and has estimates given by (10) with $\theta_0>0$, we have the important result

$$V(k'-k)/|k'|\,|k|\in\mathscr{H}\otimes\mathscr{H}. \tag{12}$$

This latter result follows from the identity

$$\iint_{\mathbf{R}^3\times\mathbf{R}^3}\frac{|V(k'-k)|^2\,dk'\,dk}{|k'|^2|k|^2}$$

$$=\iint_{\mathbf{R}^3\times\mathbf{R}^3}\frac{|V(p)|^2}{|p+k|^2|k|^2}\,dk\,dp$$

$$=J\int_{\mathbf{R}^3}\frac{|V(p)|^2}{|p|}\,dp,$$

where

$$J=2\pi\int_0^\infty\frac{1}{t}\ln\left|\frac{t+1}{t-1}\right|dt.$$

The condition that $(n^2(x)-1)$ be piecewise continuous and have compact support also will infer that the $\mathscr{D}'^m\times V(k'-k)$ satisfy conditions (11) and (12) for every finite m.

In place of conditions (11) and (12), Prosser[6] required that $V(k'-k)$ belong to a Banach space associated with condition (11), but did not include the Hilbert space given by condition (12). In addition, as will be shown next, one has to use sharper conditions on $T(k',k)$ in place of conditions (11).

For *fixed* k, the same analysis as was done for $V(k')$ can be applied to $T(k',k)$, treating it as a function of k'. It follows then that with k fixed, $T(k',k)\in C^\infty(R^3)\cap\mathscr{L}_2(R^3)$. Since $u(x,k)$ is C^2 in each domain D_i and both u and $\partial u/\partial n$ are continuous across surfaces of discontinuity in $n(x)$, one can obtain similar estimates for the behavior of $T(k',k)$ as $|k'|\to\infty$, as for $V(k')$. Thus we can conclude that as a function of k', $T(k',k)$ is bounded as follows:

$$|T(k',k)|\leqslant C(1+|k-k'|)^{-1-\theta_0},\quad k\text{ finite},$$

$$|T(k'+h',k)-T(k',k)|$$

$$\leqslant C(1+|k-k'|)^{-1-\theta_0}|h'|^\mu,\quad k\text{ finite},$$

with $|h'|<1$.

The behavior of $T(k',k)$ as a function of k and, in particular, as $(k)\to\infty$ is much more difficult to estimate. Most important when $k'=k$ (forward scattering), the behavior of $V(k'-k)$ and $T(k',k)$ are entirely different since $V(k'-k)$ becomes a constant $V(0)$, where $T(k,k)$ remains a function of k, going to zero as $(k)\to\infty$. This can be seen as follows. When $n(x)$ is sufficiently smooth, and the scattering process is sufficiently weak so that there are no caustics or multiple reflections, then $u(x,k)$ has the asymptotic form

$$u(x,k)\sim a(x)e^{i|k|\psi}[1+O(1/|k|)].$$

In the weak scattering approximations (rays approximated by straight lines) then

$$u(x,k)e^{-ik\cdot x}\sim\exp i\int^x(n(x')-1)k\cdot dx',$$

where the integral is along a line through the point x and in direction k. Upon insertion into expression (4) for $T(k',k)$ with $k'=k$, it can be seen that the resulting integral can be integrated by parts along the direction of the rays, yielding an expression that is the order of $1/|k|$.

This suggests that $T(k',k)$ has the estimating function

$$|T(k',k)|\leqslant C(1+|k'-k|)^{-1-\theta_0}(1+|k|)^{-\gamma} \tag{13a}$$

and the Hölder condition with index $\mu>\frac{1}{2}$

$$|T(k'+h',k+h)-T(k',k)|$$

$$\leqslant\frac{C[|h'|^\mu+|h|^\mu]}{(1+|k'-k|)^{1+\theta_0}(1+|k|)^\gamma}. \tag{13b}$$

An upper bound estimate for the positive constant γ will be obtained by comparing estimates of the various terms in Eq. (18). Here γ will depend upon θ_0.

Set

$$F(k',k)=k^2\int\frac{V(k'-p)T(p,k)dp}{p^2-k^2-i0}. \tag{14}$$

It can be shown (see the Appendix), that if $V(k'-k)$ and $T(k',k)$ satisfy the respective Hölder conditions (11) and (13), with Holder indices $\mu>\frac{1}{2}$, then

$$|F(k',k)|\leqslant C(1+|k'-k|)^{-1-\theta_0}(1+|k|)^{2-\theta'-\gamma},$$

and

$$|F(k'+h',k+h)-F(k',k)|$$

$$\leqslant\frac{C[|h'|^{1/2}+|h|^{1/2}]}{(1+|k'-k|)^{1+\theta_0}(1+|k|)^{-5/2+\theta'+\gamma}},$$

where $\theta'<\theta_0$ but can be made as close to θ_0 as possible.

It can now be seen, using the above estimate for expression (14), that in order for Eq. (8) to be satisfied with a positive value of γ it must have the following upper bound [if $V(0)\neq0$]:

$$\gamma+\theta_0\leqslant\tfrac{5}{2}+0. \tag{15}$$

As pointed out earlier, $T(k',k)$, as a function of the variable k', is $C^\infty(\mathbb{R}^3)$. In fact it can be shown that $\mathscr{D}^{m'}T(k',k)\in\mathscr{L}_2(\mathbb{R}^3)$ (where the prime indicates differentiation with respect to k'). Furthermore $\mathscr{D}^{m'}T(k',k)$ can be obtained from $T(k',k)$ and $\mathscr{D}^{m'}V(k'-k)$ through the following relation obtained by differentiation of Eq. (8):

$$\mathscr{D}^{m'}T(k',k)=\mathscr{D}^{m'}V(k'-k)+k^2\int\frac{\mathscr{D}^{m'}V(k'-p)T(p,k)dp}{p^2-k^2-i0}. \tag{16}$$

The interchange of the order of integration and differentiation can be justified using the Hölder conditions.

It should be pointed out in addition that it can be shown that $T(k',k)/|k'|\,|k|\in\mathscr{H}\otimes\mathscr{H}$.

IV. NECESSARY AND SUFFICIENT CONDITIONS ON $T(k',k)$

Here we want to establish certain properties of $T(k',k)$ arising from it being a solution of Eq. (8). Some of the results

that are derived here may hold for less restricted conditions on $V(k)$ or $n^2(x)-1$; however, the reality condition on $n^2(x)-1$ is essential. As a first step we want to prove the subsequent fundamental Lemma. Its proof depends upon two main properties of $V(k'-k)$ as a function of the two variables k' and k; namely, the following reality and translation invariance relations holding for all $k,k'\in\mathbb{R}^3$:

(i) $\varphi(k',k)=\bar{\varphi}(k,k')$ (reality),

(ii) $\varphi(k'+h,k+h)=\varphi(k',k)$, for all $h\in\mathbb{R}^3$.

Lemma 1: If $V(k)\in C^\infty(R^3)\cap\mathscr{L}_2(\mathbb{R}^3)$ and satisfies the Hölder estimates (10), then the solution $T(k',k)$ of Eq. (8) satisfies the relation

$$\overline{T}(k-h,k')+k^2\int\frac{T(p,k)\overline{T}(p-h,k')dp}{p^2-k^2-i0}=T(k'+h,k)+k'^2\int\frac{\overline{T}(p,k')T(p+h,k)dp}{p^2-k'^2+i0}, \tag{17}$$

for all $k,k',h\in\mathbb{R}^3$.

Proof: First make the transformations $k'\to q+h$, $k\to k+h$, $p\to p+h$ in Eq. (8) and employ the reality and the translation invariance properties on $V(k'-k)$ to obtain

$$T(q+h,k+h)=V(q-k)+|k+h|^2\int\frac{V(q-p)T(p+h,k+h)dp}{|p+h|^2-|k+h|^2-i0}. \tag{18}$$

In a similar manner, use the transformation $k'\to k$, $k\to k'$, $i\to -i$ in Eq. (8) and the before-mentioned properties of $V(k'-k)$ to yield

$$\overline{T}(k,k')=V(k'-k)+k'^2\int\frac{V(p-k)\overline{T}(p,k')dp}{p^2-k'^2+i0}. \tag{19}$$

Then operate on Eq. (18) with

$$k'^2\int\frac{\overline{T}(q,k')\cdots dq}{q^2-k'^2+i0}.$$

The resulting left-hand and right-hand sides become, respectively,

$$k'^2\int\frac{\overline{T}(q,k')T(q+h,k+h)dq}{q^2-k'^2+i0} \tag{20}$$

and

$$k'^2\int\frac{V(q-k)\overline{T}(q,k')dq}{q^2-k'^2+i0}+|k+h|^2\int\frac{T(p+h,k+h)k'^2}{|p+h|^2-|k+h|^2-i0}\times\int\frac{V(q-p)\overline{T}(q,k')dq\,dp}{q^2-k'^2+i0}. \tag{21}$$

Here the change in the order of integration can be justified by first replacing terms $q^2-k'^2+i0$ and $|p+h|^2-|k+h|^2-i0$, respectively, by $q^2-k'^2+i\epsilon_1$ and $|p+h|^2-|k+h|^2-i\epsilon_2$, where ϵ_1,ϵ_2 are small positive quantities, then interchanging the order of integration using the Hölder properties (13) of $T(k',k)$ and finally taking the limit as the ϵ's$\to 0$.

Using Eq. (19), expression (21) reduces to

$$\overline{T}(k,k')-V(k'-k)+|k+h|^2\times\int\frac{T(p+h,k+h)[\overline{T}(p,k')-V(k'-p)]dp}{|p+h|^2-|k+h|^2-i0},$$

which in turn can be reduced further [on using Eq. (18)] to

$$\overline{T}(k,k')-T(k'+h,k+h)+|k+h|^2\int\frac{T(q,k+h)\overline{T}(q-h,k')dq}{q^2-|k+h|^2-i0}.$$

Equation (17) is obtained by equating the above expression to expression (20), then replacing k by $k-h$.

Lemma 2: If $T(k',k)$ satisfies the Hölder conditions (13) and Eq. (17), then $T(k',k)$ satisfies Eq. (8) with

$$V(k'-k)=T(k'-k,0). \tag{22}$$

Proof: Set $k=k'=0$ in Eq. (17) to give

$$T(h,0)=\overline{T}(-h,0).$$

Then set $k'=0$ in Eq. (17) and use the above result in the form $\overline{T}(k-h,0)=T(h-k,0)$ to obtain

$$T(h-k,0)+k^2\int\frac{T(h-p,0)T(p,k)dp}{p^2-k^2-i0}=T(h,k).$$

This is the same as Eq. (8) if one sets $V(k'-k)=T(k'-k,0)$.

V. THE OPERATOR $\mathfrak{T}$

Define the integral operator $\mathfrak{T}$ by

$$\mathfrak{T}_k\phi=\int\frac{|k||p|T(p,k)\phi(p)dp}{p^2-k^2-i0} \tag{23}$$

with domain, the dense set of functions $\phi(k)\in\mathscr{H}$ satisfying the Hölder conditions with $\frac{1}{2}<\mu<1$,

$$\begin{aligned}&||k|\phi(k)|<C(1+|k|)^{-\beta}\\&||k+h|\phi(k+h)-|k|\phi(k)|\\&\quad<C(1+|k|)^{-\beta}|h|^{\mu},\quad |h|<1.\end{aligned} \tag{24}$$

It can be shown, using the Hölder conditions on $T(k',k)$ given by Eqs. (13), that $\mathfrak{T}_k\phi$ has the properties (see the Appendix)

$$\begin{aligned}&||k|\mathfrak{T}_k\phi|<C(1+|k|)^{-\beta'},\\&||k+h|\mathfrak{T}_{k+h}\phi-|k|\mathfrak{T}_k\phi|<C(1+|k|)^{-\beta'}|h|^{1/2},\end{aligned} \tag{25}$$

where $\beta'=\gamma+\theta_0+\beta-\frac{5}{2}-0$. It follows that for β sufficiently large, $\mathfrak{T}\phi\in\mathscr{H}$.

The adjoint operator $\mathfrak{T}^*$ is given by

$$\mathfrak{T}_k^*\phi=\int\frac{|k||p|\overline{T}(k,p)\phi(p)dp}{k^2-p^2+i0}. \tag{26}$$

For the case when $\mathfrak{T}$ operates on a function $\phi(k',k)$ of two variables the following notation will be employed to des-

ignate which variable is treated as a constant:

$$(\mathfrak{I}+\mathfrak{T}_k)_p\phi(k',p) = \phi(k',k) + \int \frac{|k|\,|p|T(p,k)\phi(k',p)dp}{p^2-k^2-i0}.$$

Theorem: If the operator $\mathfrak{T}$ defined by Eq. (23) is such that $T(k',k)$ satisfies the conditions of Lemma 1, then

$$(\mathfrak{I}+\mathfrak{T})(\mathfrak{I}+\mathfrak{T}^*) = \mathfrak{I}. \tag{27}$$

Proof: It follows immediately from Eq. (17) with $h=0$ that

$$T(k',k) - \overline{T}(k',k) = \int \frac{\overline{T}(p,k')T(p,k)[(k^2-k'^2)p^2 + i0(k^2+k'^2)]dp}{(p^2-k^2-i0)(p^2-k'^2+i0)}, \tag{28}$$

and since the right-hand side of Eq. (28) can be shown to be equivalent to

$$(k^2-k'^2+i0)\int \frac{\overline{T}(p,k')T(p,k)\,p^2dp}{(p^2-k^2-i0)(p^2-k'^2+i0)},$$

Eq. (28) reduces to

$$\frac{T(k',k)}{k'^2-k^2-i0} + \frac{\overline{T}(k,k')}{k^2-k'^2+i0} + \int \frac{p^2\overline{T}(p,k')T(p,k)dp}{(p^2-k^2-i0)(p^2-k'^2+i0)} = 0. \tag{29}$$

It is seen that if Eq. (29) is multiplied by $|k|\,|k'|$, then the resulting left-hand side is the kernel of the operator $\mathfrak{T}+\mathfrak{T}^*+\mathfrak{T}\mathfrak{T}^*$. Hence it follows that

$$\mathfrak{T}+\mathfrak{T}^*+\mathfrak{T}\mathfrak{T}^*=0,$$

and the results given by Eq. (27) are obtained.

The result of this is that $\mathfrak{I}+\mathfrak{T}^*$ is the right inverse of $\mathfrak{I}+\mathfrak{T}$. This depends upon the result, namely Eq. (17) of Lemma 1, being valid for the case $h=0$ only, which corresponds to the reality condition on $V(k',k)$.

The question now arises as to whether or not $\mathfrak{I}+\mathfrak{T}^*$ is the left inverse of $\mathfrak{I}+\mathfrak{T}$. To examine this, set

$$(\mathfrak{I}+\mathfrak{T}^*)(\mathfrak{I}+\mathfrak{T}) = \mathfrak{P} = \mathfrak{I}-\mathfrak{Q}, \tag{30}$$

$$-\mathfrak{Q} = \mathfrak{T}+\mathfrak{T}^*+\mathfrak{T}^*\mathfrak{T}. \tag{31}$$

It can be seen using Eq. (27) that

$$\mathfrak{P}^2=\mathfrak{P}, \quad \mathfrak{P}^*=\mathfrak{P}, \tag{32}$$

hence as expected, $\mathfrak{P}$ is a projection operator. Thus it follows that

$$\mathfrak{Q}^2=\mathfrak{Q}, \quad \mathfrak{Q}^*=\mathfrak{Q}. \tag{33}$$

This immediately says that $\mathfrak{Q}$ has eigenvalues 0 and $+1$. From Eqs. (27), (30), and (33) it can be deduced that

$$(\mathfrak{I}+\mathfrak{T})\mathfrak{Q} = \mathfrak{Q}(\mathfrak{I}+\mathfrak{T}^*) = 0. \tag{34}$$

The operator $\mathfrak{Q}$ can be expressed directly in terms of an integral operator

$$\mathfrak{Q}_k u = \int Q(p,k)u(p)dp, \tag{35}$$

where the kernel $Q(k',k)$ is given explicitly by the following relation:

$$(k'^2-k^2-i0)Q(k',k)/|k|\,|k'| = -T(k',k) + \overline{T}(k,k') + \int \overline{T}(k,p)T(k',p) \times\left[\frac{-k^2}{k^2-p^2+i0} + \frac{k'^2}{k'^2-p^2-i0}\right]dp. \tag{36}$$

When $|k| = |k'|$, it is seen that the right-hand side of Eq. (36) reduces to

$$-T(k',k) + \overline{T}(k,k') + \pi i|k|^3\int_\Omega \overline{T}(k,p)T(k',p)d\Omega_p,$$

where the integral is over the unit sphere, and $|p| = |k|$. Using the well-known[2] reciprocity result $T(k',-k) = T(k,-k')$ (valid for $|k| = |k'|$) and Eq. (17) with $h=0$, $|k| = |k'|$, it can be shown that the above expression vanishes. Thus the right-hand side of Eq. (36) vanishes when $|k| = |k'|$, and the kernel $Q(k',k)$ does not have a principle-value-type singularity. Because of the Hölder conditions, the singularity is like $||k'|^2 - |k|^2|^{\mu-1}$.

Unfortunately, it appears that under the estimates on $V(k'-k)$ and $T(k',k)$ imposed here, $Q(k',k)$ is not the kernel of a compact operator. One needs larger values of θ_0 and γ. If $Q(k',k)$ were compact, then one could conclude that $\mathfrak{Q}$ (being a self-adjoint operator with nonzero eigenvalue 1) would have finite rank,[9] and hence have the form

$$\mathfrak{Q}_k u = \sum_{n=1}^{N} \psi_n(k)\int \bar{\psi}_n(p)u(p)dp.$$

Here $\{\psi_n\}_{n=1}^N$ is an orthonormal set of eigenfunctions of $\mathfrak{T}$ corresponding to the eigenvalue of 1. It would then follow from Eqs. (27) and (30) that $(\mathfrak{I}+\mathfrak{T})\psi_n = 0$.

For a good part of the remainder of this paper we will be interested in the case where $\mathfrak{I}+\mathfrak{T}^*$ is the left inverse of $\mathfrak{I}+\mathfrak{T}$ occurring when $\mathfrak{Q}=0$ or when the null space of $\mathfrak{I}+\mathfrak{T}$ is empty. The condition for this to hold follows from setting $Q(k',k)=0$ in expression (36), and is given in the following lemma.

Lemma 3: If $T(k',k)$ satisfies the condition

$$T(k',k) - \overline{T}(k,k') = \int \overline{T}(k,p)T(k',p) \times \left[\frac{k'^2}{k'^2 - p^2 - i0} - \frac{k^2}{k^2 - p^2 + i0}\right] dp, \tag{37}$$

then the null space of $\Im + \mathfrak{T}$ is empty and $\Im + \mathfrak{T}$ is a unitary operator.

VI. INVERSION OF EQ. (8) WHEN $\Im + \mathfrak{T}$ IS UNITARY

In Sec. IV, necessary conditions on $T(k',k)$ were developed to ensure that $T(k',k)$ be a solution of the direct scattering problem associated with Eq. (8), where $V(k)$ is the transform of a real-valued quantity with certain smoothness. The results are stated in Lemma 1, and subsequent operator relations arising from this are given by Eqs. (27) and (30). Here we want to examine the inversion of Eq. (8) using the operator relations for the case where the $T(k',k)$ satisfies Eq. (37) as well as Eq. (17). The inversion problem can be stated as follows.

Problem P: Given that $T(k',k)$ satisfies the Hölder conditions (13), and relations (17) and (37), find a solution $v(k',k)$ of the equation

$$(\Im + \mathfrak{T}_k)_p \frac{v(k',p)}{|k'|\,|p|} = \frac{T(k',k)}{|k'|\,|k|}, \tag{38}$$

such that $v(k',k)$ satisfies the Hölder relations (11) [and, as a consequence, the condition $v(k',k)/|k'|\,|k| \in \mathscr{H} \otimes \mathscr{H}$].

It immediately follows that since $T(k',k)$ satisfies Eq. (37) the null space of $\Im + \mathfrak{T}$ is empty, hence the solution of Eq. (38) is uniquely given by

$$\frac{v(k',k)}{|k'|\,|k|} = (\Im + \mathfrak{T}_k^*)_p \frac{T(k',p)}{|k'|\,|p|}. \tag{39}$$

This can be written in the form

$$v(k',k) = T(k',k) + k^2 \int \frac{\overline{T}(k,p)T(k',p)dp}{k^2 - p^2 + i0}. \tag{40}$$

From the Appendix [see Eq. (10) and the following material], it is seen that the second term in Eq. (40) is Hölder continuous with index $\frac{1}{2}$ and estimating function $(1 + |k - k'|)^{-1-\theta_0}$, provided that γ in the Hölder conditions (13) is chosen so that $2\gamma + \theta_0 > \frac{3}{2} + 0$. As a result, from these conditions (13) applied to the first term of Eq. (40), it follows that $v(k',k)$ given by Eq. (40) satisfies Hölder estimates (11).

Next we want to examine expression (39) to see if it satisfies the reality and translation invariance condition. First note that condition (17) can be written in operator form:

$$(\Im + \overline{\mathfrak{T}}_{k'})_p \frac{T(p+h,k)}{|p|\,|k|} = (\Im + \mathfrak{T}_k)_p \frac{\overline{T}(p-h,k')}{|p|\,|k'|}. \tag{41}$$

Then operate on Eq. (41) with $(\Im + \overline{\mathfrak{T}}_{k'}^*)(\Im + \mathfrak{T}_k^*)$ using Eq. (27) and (30) (with $\Omega \equiv 0$) to yield

$$(\Im + \mathfrak{T}_k^*)_p \frac{T(k'+h,p)}{|k'|\,|p|} = (\Im + \overline{\mathfrak{T}}_{k'}^*)_p \frac{\overline{T}(k-h,p)}{|k|\,|p|}. \tag{42}$$

But from Eq. (39), it is seen that Eq. (42) is equivalent to

$$\frac{v(k'+h,k)}{|k'|\,|k|} = \frac{\overline{v}(k-h,k')}{|k'|\,|k|}. \tag{43}$$

With $h = 0$, Eq. (43) implies that $v(k',k)$ satisfies the reality condition $v(k',k) = \overline{v}(k,k')$ and as a consequence, the translation invariance condition $v(k'+h,k) = v(k',k-h)$.

It can be shown that if $\mathscr{D}'^m T(k',k)$ satisfies the Hölder conditions (13) then

$$\mathscr{D}'^m v(k',k) = |k|\,(\Im + \mathfrak{T}_k^*)_p \mathscr{D}'^m \frac{T(k',p)}{|p|}. \tag{44}$$

Hence we can summarize as follows.

Theorem: If $\mathscr{D}'^m T(k',k)$ satisfies Hölder conditions (13) for every finite m, $T(k',k)$ satisfies conditions (17) and (37), then the solution to Problem P given by Eq. (40), satisfies the reality and translation invariance condition, and is analytic in the first variable, with the appropriate derivatives given by Eq. (44). Here γ must be restricted by the relation $2\gamma + \theta_0 > \frac{3}{2} + 0$.

Conditions (17) and (37) constitute a set of sufficient conditions on $T(k',k)$ for the case where $\Im + \mathfrak{T}$ is a unitary operator.

VII. INVERSION WHEN THE NULL SPACE OF $\Im + \mathfrak{T}$ IS NOT EMPTY

For the case when the null space of $\Im + \mathfrak{T}$ is not empty, inversion Problem P as stated does not have a unique solution. However, it can be reformulated to have a unique solution by adding extra conditions. This formulation is presented as follows.

Problem P': Given that $T(k',k)$ satisfies the Hölder conditions (13) and relation (17), find a solution $v(k',k)$ of Eq. (38) such that it satisfies the Hölder conditions (11) [and as a consequence, the Hilbert-space condition $v(k',k)/|k'|\,|k| \in \mathscr{H} \otimes \mathscr{H}$] and the combined reality and translational invariance condition

$$v(k'-h,k) = \overline{v}(k+h,k'), \tag{45}$$

for every $k,k',h \in \mathbf{R}^3$.

We shall first show that Problem P' has a unique solution.

Lemma 4: The solution to Problem P' is unique.

Proof: If $w(k',k)$ is the solution of the homogeneous equation

$$(\Im + \mathfrak{T}_k)_p \frac{w(k',p)}{|k'|\,|p|} = 0,$$

then, on setting $k = 0$, it is seen that $w(k',0) = 0$ for all $k' \in \mathbf{R}^3$. But condition (45) implies that $w(k',k) = \overline{w}(k,k')$ and $w(k'-k,0) \equiv \overline{w}(k,k')$. Thus it follows that $w(k',k) \equiv w(k'-k,0) \equiv 0$.

Using operator conditions (27) and (30) the solution to Eq. (38) is given by

$$v(k',k) = |k|\,(\Im + \mathfrak{T}_k^*)_p \frac{T(k',p)}{|p|} + |k|\,\Omega_{k,p} \frac{v(k',p)}{|p|}, \tag{46}$$

where the second term on the right-hand side involving the operator Ω is unknown. However, the results of Lemma 4 indicate that it should be uniquely determined when condition (45) is imposed.

To investigate this, first rewrite condition (45) in the form

$$\frac{v(k'-h,k)}{|k'|\,|k|}=\frac{\bar{v}(k+h,k')}{|k'|\,|k|}, \tag{45'}$$

for which, for fixed h, both sides belong to the Hilbert space $\mathscr{H}\otimes\mathscr{H}$. (It can be shown that this follows from the required condition that either side belong to $\mathscr{H}\otimes\mathscr{H}$ when $h=0$.) This fact will be used in subsequent analyses.

Now insert expression (46) into (45') to obtain

$$(\Im+\mathfrak{T}^{*}_{k})_{p}\frac{T(k'-h,p)}{|k'|\,|p|}+\Omega_{k,p}\frac{v(k'-h,p)}{|k'|\,|p|}=(\Im+\bar{\mathfrak{T}}^{*}_{k'})_{p}\frac{\bar{T}(k'+h,p)}{|k|\,|p|}+\bar{\Omega}_{k',p}\frac{\bar{v}(k+h,p)}{|k|\,|p|}. \tag{47}$$

This will be reduced using the fact that $T(k',k)$ satisfies Eq. (17), or the equivalent form Eq. (41). As in the previous section, we operate on Eq. (41) with $(\Im+\bar{\mathfrak{T}}^{*}_{k'})(\Im+\mathfrak{T}^{*}_{k})$ using Eq. (27) and Eq. (30) with $\Omega\neq 0$, to yield

$$(\Im+\mathfrak{T}^{*}_{k})_{r}(\Im-\bar{\Omega}_{k',p})\frac{T(p-h,r)}{|p|\,|r|}=(\Im+\bar{\mathfrak{T}}^{*}_{k'})_{r}(\Im-\Omega_{k,p})\frac{\bar{T}(p+h,r)}{|p|\,|r|}. \tag{48}$$

Condition (48) can now be used to reduce Eq. (47) to the form

$$\Omega_{k,p}\left\{\frac{v(k'-h,p)}{|k'|\,|p|}-(\Im+\bar{\mathfrak{T}}^{*}_{k'})_{r}\frac{\bar{T}(p+h,r)}{|p|\,|r|}\right\}=\bar{\Omega}_{k',p}\left\{\frac{\bar{v}(k-h,p)}{|k|\,|p|}-(\Im+\mathfrak{T}^{*}_{k})_{r}\frac{T(p-h,r)}{|p|\,|r|}\right\}. \tag{49}$$

Equation (49) will now be decomposed into components belonging to various subspaces $\mathscr{H}\otimes\mathscr{H}$. Operate on Eq. (49) with the projection operator $\bar{\Omega}_{k'}\Omega_{k}$ to give

$$\Omega_{k,p}\bar{\Omega}_{k',r}\left\{\frac{v(r-h,p)-\bar{v}(p+h,r)}{|r|\,|p|}\right\}=0. \tag{50}$$

Similarly operate on Eq. (49) with the operator $(\Im-\bar{\Omega}_{k'})\Omega_{k}$ to give

$$(\Im-\bar{\Omega}_{k',r})\Omega_{k,p}\frac{v(r-h,p)}{|r|\,|p|}-\Omega_{k,p}(\Im+\bar{\mathfrak{T}}^{*}_{k'})_{r}\frac{\bar{T}(p+h,r)}{|p|\,|r|}=0. \tag{51}$$

Operating on Eq. (49) with $(\Im-\Omega_{k})\bar{\Omega}_{k'}$ will produce an equation similar to Eq. (51). Equation (47) reduces to the two equations (50) and (51).

The unknown portion of expression (46) now can be immediately obtained by first multiplying Eq. (51) by $|k'|$, then setting $|k'|=0$, yielding

$$\Omega_{k,p}\frac{v(-h,p)}{|p|}=\Omega_{k,p}\frac{\bar{T}(p+h,0)}{|p|}. \tag{52}$$

It will be expressed in a slightly different form, making use of Eq. (17) for the special case when $k'=k=0$, as follows:

$$T(-h,0)=\bar{T}(h,0). \tag{53}$$

Hence we have

$$\Omega_{k,p}\frac{v(k',p)}{|p|}=\Omega_{k,p}\frac{T(k'-p,0)}{|p|}. \tag{54}$$

It remains to be shown that Eqs. (50) and (51) are satisfied for all k, k' and h if relation (54) holds. First insert expression (54) into Eq. (50) to obtain

$$\Omega_{k,p}\bar{\Omega}_{k',r}\left\{\frac{T(r-h-p,0)-\bar{T}(p+h-r,0)}{|r|\,|p|}\right\}=0. \tag{55}$$

It is immediately seen from relation (53) that expression (55), and hence Eq. (50), is an identity and so does not yield any new condition on $T(k',k)$. Next substitute expression (54) into Eq. (51) to yield

$$\Omega_{k,p}\left\{(\Im+\bar{\mathfrak{T}}^{*}_{k'})_{r}\frac{\bar{T}(p+h,r)}{|p|\,|r|}-(\Im-\bar{\Omega}_{k',r})\frac{T(r-p-h,0)}{|r|\,|p|}\right\}=0.$$

Using the properties of the operator $(\Im-\bar{\Omega})$, this can be reduced further to

$$\Omega_{k,p}(\Im+\bar{\mathfrak{T}}^{*}_{k'})_{r}\left\{\frac{\bar{T}(p+h,r)}{|p|\,|r|}-(\Im+\bar{\mathfrak{T}}_{r})_{q}\frac{T(q-p-h,0)}{|p|\,|q|}\right\}=0. \tag{56}$$

The term in the curly brackets vanishes identically as a consequence of Eq. (17). [In Eq. (17) set $k'=0$, replace h by $p+h$ and k by r.] Hence Eq. (51) is also an identity.

We can now state that the solution of Problem P' is given by

$$v(k',k)=|k|(\Im+\mathfrak{T}^{*}_{k})_{p}\frac{T(k',p)}{|p|}+|k|\Omega_{k,p}\frac{T(k'-p,0)}{|p|}. \tag{57}$$

The results can be summarized as follows.

Theorem: If $T(k',k)$ satisfies the Hölder conditions (13) and relation (17), then the solution to Problem P' is given by Eq. (57). Furthermore if $\mathscr{D}'^{m}T(k',k)$ satisfies the Hölder conditions (13), then $\mathscr{D}'^{M}v(k',k)$ is given by

$$\mathscr{D}'^{m}v(k',k)=|k|(\Im+\mathfrak{T}^{*}_{k})_{p}\mathscr{D}'^{m}\frac{T(k',p)}{|p|}+|k|\Omega_{k,p}\mathscr{D}'^{m}\frac{T(k'-p,0)}{|p|}.$$

VIII. INVERSE SCATTERING PROBLEM

Here we formulate and briefly examine the inverse scattering problem, which is to determine $V(k)$ from knowledge of on-shell values ($|k'|=|k|$) of $T(k',k)$. As was shown in the previous sections the necessary and sufficient conditions for $T(k',k)$ to produce a solution $v(k',k)$ of Eq. (38), which satisfies the reality and translation invariance conditions, is for $T(k',k)$ to satisfy Eq. (17). This equation thus consti-

tutes a nonlinear equation for $T(k',k)$, which, if solved, would then yield a solution of the inverse scattering problem given by $V(k) = T(k,0)$. Explicitly then, the inverse scattering problem consists of solving the equation

$$T(k-h,k') + k^2 \int \frac{\overline{T}(p,k)T(p-h,k')dp}{p^2 - k^2 + i0}$$
$$= \overline{T}(k'+h,k) + k'^2 \int \frac{T(p,k')\overline{T}(p+h,k)dp}{p^2 - k'^2 - i0}, \quad \text{(I)}$$

for $T(k',k)$ given on-shell values $|k'| = |k|$ of $T(k',k)$. The index of refraction is then recovered from the relation

$$(n^2(x) - 1) = \int e^{ip\cdot x} T(p,0)dp.$$

However, system (I) is difficult to solve by iterative techniques that require the Fréchet derivative and its inverse such as Newton's methods.[10,11] This is due to the various different arguments of $T(k',k)$ appearing in system (I). A form more suitable for such analysis can be obtained by assuming differentiability of $T(k',k)$ with respect to the components $k'_j, j = 1,2,3$, of the first argument. Such an alternative form to system (I) is given by

$$(I-E)\left\{T(k',k) + k'^2 \int \frac{T(p,k)\overline{T}(p,k')dp}{p^2 - k'^2 + i0}\right\} = 0,$$
$$(I+E)\left\{\frac{\partial T(k',k)}{\partial k'_j}\right.$$
$$\left. + k'^2 \int \frac{\overline{T}(p,k')}{p^2 - k'^2 + i0} \frac{\partial T(p,k)}{\partial p_j} dp\right\} = 0, \quad \text{(I')}$$

where $j = 1,2,3$ and E stands for the operator that interchanges k and k' and takes complex conjugate of the resulting expression.

The first equation corresponds to the reality condition [given by Eq. (17) with $h = 0$]. The remaining three equations correspond to the translational invariance condition. They can be derived directly from system (I) through a limiting process in which h tends to zero. Or else, they can be derived by first expressing the translational invariance condition on $v(k',k)$ in the differential form

$$\frac{\partial}{\partial k'_j} v(k',k) + \frac{\partial}{\partial k_j} v(k',k) = 0,$$

and then modifying it using the reality condition to give

$$\frac{\partial}{\partial k'_j} v(k',k) + \frac{\partial}{\partial k_j} \overline{v}(k,k') = 0. \quad (58)$$

Then by using equations (58) in conjunction with Eq. (8), the remaining equations of system (I') can be derived in the same manner as Eq. (17) was derived in Lemma 1.

The remaining nonlinear formulations of the inverse scattering problem are obtained under the assumption that the null space of $\mathfrak{I} + \mathfrak{T}$ is empty, in which case the solution $v(k',k)$ to Eq. (58) is given by Eq. (40). Reality and translational invariance conditions are then imposed on the solution $v(k',k)$. Explicitly, the inverse scattering problem is to solve the system

$$v(k',k) = \overline{v}(k-h,k'-h), \quad k,k',h \in \mathbf{R}^3,$$
$$v(k',k) = T(k',k) + k^2 \int \frac{\overline{T}(k,p)T(k',p)dp}{k^2 - p^2 + i0}, \quad \text{(II)}$$

for $T(k',k)$, given on-shell values $|k'| = |k|$ of $T(k',k)$. The index of refraction is then recovered by noting that $v(k',k) = V(k'-k)$.

An equivalent form of system (II) more suitable for use in iteration schemes involving Fréchet derivatives can be obtained by applying the translational invariance condition on $v(k',k)$ in the form given by Eq. (58). The resulting system is

$$(I-E)\left\{T(k',k) + k^2 \int \frac{\overline{T}(k,p)T(k',p)dp}{k^2 - p^2 + i0}\right\} = 0,$$
$$(I+E)\left\{\frac{\partial T(k',k)}{\partial k'_j} + k^2 \int \frac{\overline{T}(k,p)}{k^2 - p^2 + i0} \frac{\partial T(k',p)dp}{\partial k'_j}\right\} = 0. \quad \text{(II')}$$

Since nonlinear systems have multiple solutions, one might want to include, with system (II'), the first equation of system (I').

Special nonlinear systems can be formulated that are useful when certain on-shell data is available, such as backscattered data. For instance, by employing the reality and translational invariance conditions in the form

$$v(k',k) = \tfrac{1}{2}v(k'-h,k-h) + \tfrac{1}{2}\overline{v}(k-h,k'-h), \quad (59)$$

setting $h = \frac{1}{2}(k+k')$, and inserting expression (40) into Eq. (59), one obtains the following equation:

$$T(k',k) + k^2 \int \frac{\overline{T}(k,p)T(k',p)dp}{k^2 - p^2 + i0}$$
$$= \frac{1}{2}[T(\kappa,-\kappa) + \overline{T}(-\kappa,\kappa)] + \frac{1}{2}\kappa^2 \int \overline{T}(-\kappa,p)T(\kappa,p)\left[\frac{1}{\kappa^2 - p^2 + i0} + \frac{1}{\kappa^2 - p^2 - i0}\right]dp, \quad \text{(III)}$$

where $\kappa = \frac{1}{2}(k'-k)$. The first term on the right-hand side of system (III) involves backscattered data only.

System (III) can be solved by the method of successive approximation[10,11] for solutions $T(k',k)$ belonging to the Banach space with norm

$$||T(k',k)|| = \sup_{\substack{k',k \\ |h'|<1,\ |h|<1}} \left\{\left(|T(k',k)| + \frac{|T(k'+h',k+h) - T(k',k)|}{|h'|^\mu + |h|^\mu}\right)(1 + |k'-k|)^{1+\theta_0}(1+|k|)^\gamma\right\},$$

where γ is restricted by the relation $2\gamma+\theta_0>\frac{5}{2}$. However, such an approach is valid only for very weak scattering[6] corresponding to the small norm $T(k',k)$.

IX. COMMENTS

The nonlinear systems derived in Sec. VIII need to be completely analyzed, to determine, under various circumstances, which is the best system to use to get off-shell data from on-shell. It also may be possible to derive other quadratic systems that are more practical. The analysis here can be extended to other systems. It appears noteworthy that it is applicable to Maxwell's equation.

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APPENDIX: HÖLDER CONTINUITY OF CERTAIN INTEGRALS

Let $f(k_1,k_2,k_3)$, $k_i\in\mathbb{R}^3$, be a Hölder-continuous function with indices μ_i $(i=1,2,3)$ and estimating function $M(k_1,k_2,k_3)$, i.e.,

$$|f(k_1,k_2,k_3)|\leqslant CM(k_1,k_2,k_3) \tag{A1}$$

$$|f(k_1+h_1,k_2+h_2,k_3+h_3)-f(k_1,k_2,k_3)|$$
$$\leqslant CM(k_1,k_2,k_3)\sum_{j=1}^{3}|h_j|^{\mu_j}, \tag{A2}$$

where $|h_i|\leqslant 1$. Let the integral of the estimating function over the unit sphere satisfy the inequality

$$\int M(k_1,k_2,k_3)d\Omega_3\leqslant CN(k_1,k_2)(1+|k_3|)^{-1-\theta}, \tag{A3}$$

then[1] it can be shown that

$$F(k_1,k_2,z)=\int\frac{f(k_1,k_2,k_3)dk_3}{(k_3^2-z)} \tag{A4}$$

is a Hölder function for $k_1,k_2\in\mathbb{R}^3$ and z in the complex plane cut along the positive axis. Here $F(k_1,k_2,z)$ has indices μ_1', μ_2', and ν with $\mu_1'<\mu_1$, $\mu_2'<\mu_2$, and ν (the Hölder index corresponding to z) given by $\nu=\min(\frac{1}{2},\mu_3)$. The estimating function for $F(k_1,k_2,z)$ is

$$M_1(k_1,k_2,z)=N(k_1,k_2)(1+|z|)^{-\theta'/2}, \tag{A5}$$

where $\theta'<\min(1,\theta)$ can be made as close as possible to θ when $0<\theta<1$.

For the special case where $z=|k_1|^2\pm i0$, it is seen that

$$|F(k_1,k_2,|k_1|^2\pm i0)|$$
$$\leqslant C_1N(k_1,k_2(1+|k_1|^2)^{-\theta'/2}.$$

To obtain the corresponding estimates for the Hölder indices, note that for $|h|\leqslant 1$

$$|F(k_1,k_2,|k_1+h|^2\pm i0)-F(k_1,k_2,|k_1|^2)|$$
$$\leqslant CN(k_1,k_2)|h^2+2k_1\circ h|^{\nu}$$
$$\leqslant C_0N(k_1,k_2)(1+|k_1|)^{\nu}|h|^{\nu}.$$

From this it is seen that $F(k_1,k_2,|k_1^2|\pm i0)$ is a Hölder function for $k_i\in\mathbb{R}^3$, with indices $\mu_1''=\min[\mu_1',\frac{1}{2},\mu_3]$, $\mu_2''=\mu_2'$, and the estimating function

$$M_2(k_1,k_2)\leqslant N(k_1,k_2)(1+|k|)^{\nu-\theta'}, \tag{A6}$$

where $\theta'<\min[1,\theta]$.

To obtain the estimate (A3) for the various estimating functions in this paper we require the following inequalities that are found in Faddev[1]:

$$(1+|k-p|)^{-\theta}(1+|k'-p|)^{-\theta}$$
$$\leqslant C[(1+|k-p|)^{-\theta}$$
$$+(1+|k'-p|)^{-\theta}](1+|k-k'|)^{-\theta}, \tag{A7}$$

valid for $0<\theta$; and

$$\int(1+|k-p|)^{-\theta}d\Omega_p$$
$$\leqslant C(1+|k|)^{-\theta_1}(1+|p|)^{-\theta_2},$$
$$\theta_1+\theta_2=\theta<2. \tag{A8}$$

Combining the results of (A6)–(A8), with $\theta_1=0$ and $\theta_2=\theta$, it can be seen that since $V(k'-p)T(p,k)$ has the estimating function

$$(1+|k'-p|)^{-1-\theta_0}(1+|k-p|)^{-1-\theta_0}(1+|k|)^{-\gamma}$$

and Hölder indices $\mu_i>\frac{1}{2}$, then

$$k^2\int\frac{V(k'-p)T(p,k)dp}{p^2-k^2-i0}$$

is Hölder continuous with the estimating function

$$(1+|k'-k|)^{-1-\theta_0}(1+|k|)^{5/2-\gamma-\theta'},$$

where θ' can be made as close as possible to θ_0.

The corresponding Hölder estimates for the operator given by Eq. (23) are similarly obtained noting that $T(p,k)|p|\phi(p)$ is Hölder continuous with indices $>\frac{1}{2}$, and estimating function

$$(1+|p-k|)^{-1-\theta_0}(1+|k|)^{-\gamma}(1+|p|)^{-\beta}.$$

Hence using expressions (A6) and (A8), the Hölder estimating function is obtained:

$$\left|\int\frac{T(p,k)|p|\phi(p)dp}{p^2-k^2-i0}\right|\leqslant C(1+|k|)^{1/2-\gamma-\theta'-\beta}, \tag{A9}$$

where $\theta'<\theta_0$.

To obtain the Hölder estimates for the function

$$\int\frac{k^2\overline{T}(k,p)T(k',p)dp}{k^2-p^2+i0}, \tag{A10}$$

it should first be decomposed into two parts:

$$\int\overline{T}(k,p)T(k',p)dp+\int\frac{p^2\overline{T}(k,p)T(k',p)dp}{k^2-p^2+i0}. \tag{A11}$$

Noting that $p^2\overline{T}(k,p)T(k',p)$ has the estimating function

$$(1+|k-p|)^{-1-\theta_0}(1+|k'-p|)^{-1-\theta_0}$$
$$(1+|p|)^{-2\gamma+2},$$

it can be shown, using (A7) and (A8) with $\theta_1=0$ and $\theta_2=1+\theta_0$, that the first integral in expression (A11) is Hölder continuous with estimating function $(1+|k-k'|)^{-1-\theta_0}$ provided that $2\gamma+\theta_0-2>0$. Again, using Eqs. (A6)–(A8) with $\theta_2=1+\theta_0$, it can be shown that the second integral in expression (A11) is Hölder continuous with indices $>\frac{1}{2}$, and estimating function

$$(1+|k-k'|)^{-1-\theta_0}(1+|k|)^{1/2-\theta'},$$

where

$$\theta' = <\text{Min}[1,2\gamma-2+\theta_0].$$

Hence it can be seen that expression (A10) is Hölder continuous with estimating function $(1+|k-k'|)^{-1-\theta_0}$ provided that γ is chosen so that $2\gamma+\theta_0>\frac{5}{2}+0$.

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Discrete quantum mechanics

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A discrete model for quantum mechanics is presented. First a discrete phase space S is formed by coupling vertices and edges of a graph. The dynamics is developed by introducing paths or discrete trajectories in S. An amplitude function is used to compute probabilities of quantum events and a discrete Feynman path integral is presented. Many of the results can be formulated in terms of transition probabilities and unitary operators on a Hilbert space $l^2(S)$.

I. INTRODUCTION

Modern quantum theory appears to have reached a stage similar to its beginnings when Planck postulated his quantum action principle. This principle stated that radiation of a given frequency ν could only exist in discrete energy packets with values $nh\nu$, $n = 1,2,\ldots$. Of course, Planck's postulate was necessary to circumvent the ultraviolet catastrophe of classical mechanics that predicted an infinite energy for a radiating body. The situation is similar in the modern theories of QED, QCD, and their more rigorous versions, quantum field theory and gauge field theory. The former theories are plagued with infinities and singularities, while the latter lack concrete physical models and predictive power. Some investigators believe that these theories break down at small distances or high energies because they are based upon a continuum model of space-time.[1–5] These theories cannot succeed because space-time is not a continuum but is discrete. There exists in nature an elementary length and an elementary time and all length and time measurements must be integer multiples of these.[6–12]

In this paper, we present a discrete model for quantum mechanics that might be called quantum graphicdynamics (QGD). The first stage of the model is a graph G that represents discrete locations for a particle. A discrete phase space S is formed by coupling vertices and edges of G. Quantum mechanics comes into play by postulating an amplitude function $A: S \times S \to \mathbb{C}$, which gives the amplitude that a particle can move from one point in S to another in one discrete time step. The dynamics is developed by introducing paths or discrete trajectories in S. The amplitude of a path is defined as the product of the amplitudes of its one-step parts. By summing the amplitudes of various paths and taking the modulus squared of this sum, we obtain the quantum probability of events. This is the discrete analog of the Feynman path integral, and results in a quantum random walk. This theory not only describes an evolution in discrete space-time, it may also be useful for models in which a composite particle is described by a finite graph, whose vertices represent elementary particles such as quarks.

In the following section we develop the general theory of QGD. Free and perturbed amplitude functions are introduced. It is shown that amplitude functions give a transition probability on a Hilbert space $l^2(S)$ over the discrete phase-space S. Moreover, it is shown that dynamical propagators are given by unitary operators on $l^2(S)$. A relationship between free and perturbed propagators is derived. In Sec. III, simplifying assumptions are made and the theory is specialized to infinite square lattices. In Secs. IV and V, concrete examples are discussed in low-dimensional lattices and finite graphs, respectively.

Some other approaches to discrete quantum mechanics, which are quite different from that presented here, may be found in Refs. 13–17.

II. GENERAL THEORY

In this paper a *graph* is a pair $G = (V,E)$, where V is an arbitrary nonempty set and E is a collection of two element subsets of V. The elements of V are called *vertices* and the elements of E are called *edges*. Suppose that $V = \{v_j : j \in J\}$ and that the edges containing v_j are denoted by e_{jk}, $k \in K(j)$. If $\{v_r, v_s\} \in E$ we write $v_r \perp v_s$ and say that v_r, v_s are *adjacent*. The *phase space* on G is the set

$$S = \{(v_j, e_{jk}) : j \in J,\ k \in K(j)\} \subseteq V \times E.$$

If $q = (v_j, e_{jk}) \in S$, $q' = (v_{j'}, e_{j'k'}) \in S$ and $v_j \perp v_{j'}$, we write $q \perp q'$. For $n \in \mathbb{N}$, an *n-path* is a sequence of not necessarily distinct elements $q_0,\ldots,q_n \in S$ with $q_j \perp q_{j+1}$, $j = 0,\ldots,n-1$. We call q_0, q_n the *initial* and *final* elements, respectively, of the n-path. Denote the set of n-paths with initial element q_0 and final element q by $\mathscr{P}_n(q_0,q)$. Physically, we think of V as a set of discrete position coordinates for a particle and adjacent vertices correspond to "nearest neighbor" positions. An edge containing $v \in V$ corresponds to a direction that a particle located at v can move and hence represents a momentum (the magnitude will be added as a parameter later). If $e = \{v_1, v_2\} \in E$, then a particle located at v_1 can move along e to v_2 in one time step. An n-path $p \in \mathscr{P}_n(q_0,q)$ is a possible trajectory for a particle moving in a discrete phase space from q_0 to q in n time steps.

A function $A: S \times S \to \mathbb{C}$ is an *amplitude function* if $A(q,q') = 0$ if $q \not\perp q'$ and for all $q_1, q_2 \in S$ we have

$$\sum_{q'} A(q_1,q')\overline{A}(q_2,q') = \sum_{q'} A(q',q_1)\overline{A}(q',q_2) = \delta_{q_1,q_2}, \qquad (1)$$

where $\overline{A}$ denotes the complex conjugate of A. We then call (G,A) an *amplitude graph*. If

$$p = \{q_0,\ldots,q_n\} \in \mathscr{P}_n(q_0,q)$$

the *amplitude* of p is defined by

$$A(p) = A(q_0,q_1)A(q_1,q_2)\cdots A(q_{n-1},q_n). \qquad (2)$$

For $q_0, q \in S$, the *n-step transition amplitude of* q_0 *to* q is

$$A_n(q_0,q) = \sum \{A(p) : p \in \mathscr{P}_n(q_0,q)\}, \qquad (3)$$

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and by convention $A_0(q_0,q)=\delta_{q_0q}$. Notice that $A_1(q_0,q)=A(q_0,q)$. The *n-step transition probability of* q_0 *to* q is $P_n(q_0,q)=|A_n(q_0,q)|^2$. Moreover, for $v_j\in V$ we define

$$A_n(q_0,v_j)=\sum\{A(p):p\in\mathscr{P}_n(q_0,q),\ q=(v_j,e_{jk}),\quad k\in K(j)\},$$

$$P_n(q_0,v_j)=|A_n(q_0,v_j)|^2.$$

We now give physical interpretations for the definitions in the previous paragraph. We interpret $A(q,q')$ as a probability amplitude that a particle moves from q to q' in one time step. The corresponding probability is $P(q,q')=|A(q,q')|^2$. The first condition means that if q and q' are not nearest neighbors, then a particle cannot move from q to q' in one time step. If $q_1=q_2$, then Eq. (1) gives

$$\sum_{q'}P(q_1,q')=\sum_{q'}P(q',q_1)=1.$$

The first summation states that a particle beginning at q_1 must move to a nearest neighbor after one time step, and the second summation states that a particle ending at q_1 must have begun at a nearest neighbor one time step previously. As we shall later show, Eq. (1) is equivalent to the existence of a unitary propagator T on a Hilbert space H. Moreover, any $q\in S$ corresponds to a unit vector $\delta_q\in H$ and $A(q,q')=\langle T\delta_q,\delta_{q'}\rangle$.

For $q_1\neq q_2$, Eq. (1) gives

$$\langle\delta_{q_1},\delta_{q_2}\rangle=\langle T\delta_{q_1},T\delta_{q_2}\rangle=\sum_{q'}\langle T\delta_{q_1},\delta_{q'}\rangle\langle\delta_{q'},T\delta_{q_2}\rangle=0,$$

so q_1 and q_2 correspond to orthogonal states. We can then interpret Eq. (1) as meaning that a particle cannot simultaneously be at two different points in S. Equation (2) is a Markov property for the amplitude of a trajectory, and Eq. (3) states that $A_n(q_0,q)$ is the sum of the amplitude for all n-step trajectories from q_0 to q.

In the following theorem, (a) shows that probability is conserved after n time steps and (b) is the discrete Chapman–Kolmogorov equation.

Theorem 1:

(a) $\sum_q|A_n(q_0,q)|^2=1.$

(b) If $m,n\in\mathbf{N}$ with $m\leqslant n$, then

$$A_n(q_0,q)=\sum_{q'}A_m(q_0,q')A_{n-m}(q',q).\tag{4}$$

Proof: It is clear that (4) holds if $m=n$, so assume that $m<n$. We prove (a) and (b) by induction on n. For $n=1$, (a) holds by Eq. (1). For $n=2$, we have

$$A_2(q_0,q)=\sum\{A(p):\ p\in\mathscr{P}_2(q_0,q)\}$$

$$=\sum_{q'}A_1(q_0,q')A_1(q',q),$$

so (b) holds for $n=2$. Moreover, the sum converges absolutely since by Schwarz's inequality

$$\sum_{q'}|A(q_0,q')A(q',q)|$$

$$<\left[\sum_{q'}|A(q_0,q')|^2\sum_{q'}|A(q',q)|^2\right]^{1/2}=1.$$

It now follows from (1) that

$$\sum_q|A_2(q_0,q)|^2=\sum_q\sum_{q'}A(q_0,q')A(q',q)\times\sum_{q''}A(q_0,q'')A(q'',q)$$

$$=\sum_{q',q''}A(q_0,q)A(q_0,q'')\times\sum_qA(q',q)A(q'',q)$$

$$=\sum_{q',q''}A(q_0,q')A(q_0,q'')\delta_{q'q''}=1.$$

Hence, (a) holds for $n=2$. Now suppose that (a) and (b) hold for $n=2,3,\ldots,r$ and let $n=r+1$, $m<n$. Then

$$A_{r+1}(q_0,q)=\sum\{A(p):p\in\mathscr{P}_{r+1}(q_0,q)\}$$

$$=\sum_{q'\mathrm{l}q}\sum\{A(p')A(q',q):p'\in\mathscr{P}_r(q_0,q')\}$$

$$=\sum_{q'\mathrm{l}q}A(q',q)\sum\{A(p'):p'\in\mathscr{P}_r(q_0,q')\}$$

$$=\sum_{q'}A_1(q',q)A_r(q_0,q').$$

Hence, (b) holds for $m=r$. Moreover, using the induction hypothesis and proceeding as before, the sum converges absolutely and

$$\sum_q|A_{r+1}(q_0,q)|^2=1.$$

Hence, (a) holds for $n=r+1$. Finally, if $m<r$ we have, by the induction hypothesis,

$$A_{r+1}(q_0,q')=\sum_{q'}A_1(q',q)A_r(q_0,q')$$

$$=\sum_{q'}A_1(q',q)\sum_{q''}A_m(q_0,q'')A_{r-m}(q'',q)$$

$$=\sum_{q''}A_m(q_0,q'')\sum_{q'}A_{r-m}(q'',q')A_1(q',q)$$

$$=\sum_{q''}A_m(q_0,q'')A_{r+1-m}(q'',q).$$

Thus, (b) holds for $n=r+1$, and the proof is complete by induction. □

Let $l^2(S)$ be the Hilbert space of functions $\{f:\ S\to\mathbf{C}:\ \Sigma_q|f(q)|^2<\infty\}$ with inner product $\langle f,g\rangle=\Sigma f(q)\bar{g}(q)$. An orthonormal basis for $l^2(S)$ is the set $\{\delta_q:\ q\in S\}$, where $\delta_q(q')=\delta_{qq'}$. Notice that $f(q)=\langle f,\delta_q\rangle$, for every $f\in l^2(S)$, $q\in S$. It follows from (1) that $A(q_0,\cdot),A(\cdot,q_0)\in l^2(S)$ and from Theorem 1(a) that $A_n(q_0,\cdot)\in l^2(S)$. Using the usual quantum terminology, we call a unit vector $\psi\in l^2(S)$ a *state* and if ψ_1,ψ_2 are states, we call $\langle\psi_1,\psi_2\rangle$ the *transition amplitude* from ψ_1 to ψ_2. Moreover, $|\langle\psi_1,\psi_2\rangle|^2$ is the *transition probability* from ψ_1 to ψ_2. Define the linear operators T, U on $l^2(S)$ by

$$(Tf)(q) = \sum_{q'} A(q,q') f(q'),$$
$$(Uf)(q) = \sum_{q'} \overline{A}(q',q) f(q'). \tag{5}$$

We call T the *propagator* for A. It is clear that $A(q_0,q) = \langle T\delta_q, \delta_{q_0}\rangle$. It will follow from the next theorem that $T\delta_q$ is a state and hence $A(q_0,q)$ can be interpreted as the transition amplitude from this state of δ_{q_0}.

Theorem 2: The operators T and U are unitary and $U = T^*$.

Proof: To show that T is unitary, we have for $f,g \in l^2(S)$ that

$$\langle Tf, Tg\rangle = \sum_q (Tf)(q)\,\overline{(Tg)}(q)$$
$$= \sum_{q,q'} A(q,q') f(q') \sum_{q''} \overline{A}(q,q'')\bar{g}(q'')$$
$$= \sum_{q',q''} f(q')\bar{g}(q'') \sum_q A(q,q')\overline{A}(q,q'')$$
$$= \sum_{q',q''} f(q')\bar{g}(q'')\delta_{q'q''} = \langle f,g\rangle.$$

Similarly, U is unitary. To show that $U = T^*$, for $f,g \in l^2(S)$ we have

$$\langle f, Tg\rangle = \sum_q f(q)\,\overline{Tg}(q)$$
$$= \sum_q f(q) \sum_{q'} \overline{A}(q,q')\bar{g}(q')$$
$$= \sum_{q'} \bar{g}(q) \sum_q \overline{A}(q,q') f(g)$$
$$= \sum_{q'} \bar{g}(q)(Uf)(q') = \langle Uf, g\rangle. \qquad \square$$

We have seen that if A is an amplitude function, then its propagator T is unitary. We now show that the converse holds. Let A: $S \times S \to \mathbb{C}$ be a function satisfying $A(q,q') = 0$ if $q \not\perp q'$. Define the linear operator T on $l^2(S)$ by (5) and suppose that T is unitary. Then

$$\sum_{q'} A(q_1,q')\overline{A}(q_2,q')$$
$$= \sum_{q'} \langle T\delta_{q'}, \delta_{q_1}\rangle \langle \overline{T\delta_{q'}, \delta_{q_2}}\rangle$$
$$= \sum_{q'} \langle T^*\delta_{q_2}, \delta_{q'}\rangle \langle \delta_{q'}, T^*\delta_{q_1}\rangle$$
$$= \langle T^*\delta_{q_2}, T^*\delta_{q_1}\rangle = \langle \delta_{q_2}, \delta_{q_1}\rangle = \delta_{q_1,q_2}.$$

In a similar way, the other equality in (1) holds so that A is an amplitude function.

For $f \in l^2(S)$ we define $A_n(f|q_0) = \Sigma_q f(q) A_n(q_0,q)$, $A_0(f|q_0) = f(q_0)$. Notice that $A_n(\cdot|q_0)$ is a bounded linear functional and that $A_n(\delta_q|q_0) = A_n(q_0,q)$. Moreover, $A_1(f|q_0) = Tf(q_0)$. For f: $S \to \mathbb{R}$ we define the *n-step expectation* $E_n(f|q_0) = \Sigma_q f(q) P_n(q_0,q)$ provided that the sum converges.

Theorem 3: For $f \in l^2(S)$, we have $A_n(f|q_0) = T^n f(q_0)$.

Proof: Proceeding by induction on n, the result holds for $n = 1$. Suppose the result holds for n and apply Theorem 1(b) to obtain

$$A_{n+1}(f|q_0) = \sum_q f(q) \sum_{q'} A_1(q_0,q') A_n(q',q)$$
$$= \sum_{q'} A(q_0,q') \sum_q f(q) A_n(q',q)$$
$$= \sum_{q'} A(q_0,q') A_n(f|q')$$
$$= TA_n(f|q_0) = T^{n+1} f(q_0). \qquad \square$$

Corollary 4: $A_n(q_0,q) = \langle \delta_q, U^n \delta_{q_0}\rangle$.

Proof: Applying Theorem 3 gives

$$A_n(q_0,q) = A_n(\delta_q|q_0) = T^n\delta_q(q_0) = \langle T^n\delta_q, \delta_{q_0}\rangle$$
$$= \langle \delta_q, (T^n)^*\delta_{q_0}\rangle = \langle \delta_q, U^n\delta_{q_0}\rangle. \qquad \square$$

Let P_q be the one-dimensional projection onto the unit vector $\delta_q \in l^2(S)$. For f: $S \to \mathbb{R}$, define the self-adjoint operator B_f on $l^2(S)$ by $B_f g(q) = f(q)g(q)$. Then B_f has the representation $B_f = \Sigma_q f(q) P_q$. The next corollary gives the usual quantum probabilities and expectations.

Corollary 5:

(a) $P_n(q_0,q) = \langle P_q U^n \delta_{q_0}, U^n\delta_{q_0}\rangle$.

(b) $E_n(f|q_0) = \langle B_f U^n\delta_{q_0}, U^n\delta_{q_0}\rangle$.

Proof:

(a) $P_n(q_0,q) = |\langle \delta_q, U^n\delta_{q_0}\rangle|^2 = \langle P_q U^n\delta_{q_0}, U^n\delta_{q_0}\rangle$.

(b) $E_n(f|q_0) = \sum f(q) P_n(q_0,q)$
$$= \sum f(q) \langle P_q U^n\delta_{q_0}, U^n\delta_{q_0}\rangle$$
$$= \left\langle \sum f(q) P_q U^n\delta_{q_0}, U^n\delta_{q_0}\right\rangle$$
$$= \langle B_f U^n\delta_{q_0}, U^n\delta_{q_0}\rangle. \qquad \square$$

Assume that the amplitude function A corresponds to a free evolution of a particle. Now suppose that a function V: $S \to \mathbb{R}$ represents a potential energy. We then define A^V: $S \times S \to \mathbb{C}$ by $A^V(q,q') = e^{-iV(q)} A(q,q')$. Then clearly, A^V satisfies (1) so A^V is a new amplitude function. We regard A^V as the amplitude corresponding to a particle evolving under the influence of the potential V. Notice that if V is identically zero, then A^V reduces to the free amplitude function A. If $p = \{q_0,\ldots,q_n\} \in \mathscr{P}_n(q_0,q)$, then we easily obtain the Feynman-type formula

$$A^V(p) = A(p)\exp\left[-i\sum_{j=0}^{n-1} V(q_j)\right].$$

We thus obtain the following perturbed n-step transition amplitude:

$$A_n^V(q_0,q) = \sum \left\{A(p)\exp\left[-i\sum_{j=0}^{n-1} V(q_j)\right]: p = \{q_0,\ldots,q_n\} \in \mathscr{P}_n(q_0,q)\right\}.$$

Now define the unitary operator e^{-iV} by $e^{-iV} f(q) = e^{-iV(q)} f(q)$. The next corollary shows that the propaga-

tor for A^V is the unitary operator $T_V = e^{-iV}T$.

Corollary 6: (a) If T_V is the propagator for A^V, then $T_V = e^{-iV}T$.

(b) $A_n^V(q_0,q) = \langle \delta_{q'}(Ue^{iV})^n \delta_{q_0} \rangle$.

Proof: (a) By definition of the propagator for A^V, we have

$$(T_V f)(q) = \sum_{q'} A^V(q,q') f(q')$$

$$= \sum_{q'} e^{-iV(q)} A(q,q') f(q')$$

$$= e^{-iV(q)} \sum_{q'} A(q,q') f(q') = (e^{-iV} T f)(q).$$

(b) Applying Corollary 4 and (a) we have

$$A_n^V(q_0,q) = \langle T_V^n \delta_{q'} \delta_{q_0} \rangle = \langle (e^{-iV}T)^n \delta_{q'} \delta_{q_0} \rangle$$

$$= \langle \delta_q, (e^{-iV}T)^{*n} \delta_{q_0} \rangle = \langle \delta_{q'} (Ue^{iV})^n \delta_{q_0} \rangle. \quad \square$$

Let $U = \int_0^{2\pi} e^{i\theta} P(d\theta)$ be the spectral representation of U. It follows from Corollary 4 that

$$A_n(q_0,q) = \int_0^{2\pi} e^{in\theta} \langle \delta_q, P(d\theta) \delta_{q_0} \rangle.$$

Hence, there exists measures $\mu_{q_0,q}$ on $[0,2\pi]$ such that

$$A_n(q_0,q) = \int_0^{2\pi} e^{in\theta} \mu_{q_0,q}(d\theta)$$

for all $n \in \mathbb{N}$, $q_0,q \in S$. In the case that U has a complete set of eigenvectors ψ_j with corresponding eigenvalues $e^{i\lambda j}$, Corollary 4 reduces to

$$A_n(q_0,q) = \langle \delta_q, U^n \delta_{q_0} \rangle$$

$$= \left\langle \sum_j \langle \delta_q, \psi_j \rangle \psi_j, U^n \sum_{j'} \langle \delta_{q_0}, \psi_{j'} \rangle \psi_{j'} \right\rangle$$

$$= \sum_{jj'} \bar{\psi}_j(q) \psi_{j'}(q_0) \langle \psi_j, e^{in\lambda_{j'}} \psi_{j'} \rangle$$

$$= \sum_j e^{-in\lambda_j} \psi_j(q_0) \bar{\psi}_j(q).$$

III. SQUARE LATTICES

In this section we apply the general theory of Sec. II to the case of a square m-dimensional lattice $V = Z^m$, $Z = \{0, \pm 1, \pm 2, \ldots\}$. Two vertices $v_1, v_2 \in V$ are defined to be adjacent ($v_1 \perp v_2$) if one of their components differ by 1 and the others are equal. Thus, nearest neighbors in the usual sense are adjacent. Denoting the set of edges by E, we obtain a graph $G = (V,E)$. As usual, we denote the phase space on G by S. Now any $v \in V$ has $2m$ nearest neighbors and hence $2m$ incident edges. We can represent any $q \in S$ in the form

$$q = (v,s) = (j_1,\ldots,j_m,s),$$

$$s \in \{1,\ldots,2m\}, \quad j_r \in Z, \quad r = 1,\ldots,m.$$

We can represent an $f \in l^2(S)$ by $f_s(j_1,\ldots,j_m) = f(j_1,\ldots,j_m,s)$. If A: $S \times S \to \mathbb{C}$ is an amplitude function, we have

$$(Tf_s)(j_1,\ldots,j_m)$$

$$= \sum A(j_1,\ldots,j_m,s,j_1',\ldots,j_m',s') f_{s'}(j_1',\ldots,j_m').$$

We now make a simplifying assumption, which is reasonable on physical grounds. In the sequel we shall assume that A is *translation invariant*, that is, for all $k = 1,\ldots,m$.

$$A(j_1,\ldots,j_k + r,\ldots,j_m,s,j_1',\ldots,j_k' + r,\ldots,j_m',s')$$

$$= A(j_1,\ldots,j_m,s,j_1',\ldots,j_m',s')$$

$$= A(j_1,\ldots,j_m,s,j_1',\ldots,j_m',s')$$

for any $r \in Z$. Let I be the set of m-tuples $(j_1,\ldots,j_m)$, where one of the j_k equals ± 1 and the others are 0. Clearly, the cardinality $|I| = 2m$. Then A is determined by the $8m^3$ numbers

$$A(s,j,r) = A(0,\ldots,0,s,j_1,\ldots,j_m,r),$$

$$s,r = 1,\ldots,2m, \quad j = (j_1,\ldots,j_m) \in I.$$

In general, it is quite difficult to compute the value of $A_n(q_0,q)$ in a closed form. In this section we shall simplify this computation by transforming $l^2(S)$ to a new representation space. Let

$$X = [0,2\pi]^m = \{x : x = (x_1,\ldots,x_m),$$

$$x_j \in [0,2\pi], \quad j = 1,\ldots,m\}.$$

Form the Hilbert space $H = L^2(X) \otimes \mathbb{C}^{2m}$ and denote a function f in this space by $f_s(x)$, $x \in X$, $s \in \{1,\ldots,2m\}$. The inner product in H is taken to be

$$\langle f,g \rangle = \frac{1}{(2\pi)^m} \int_0^{2\pi} f \cdot g \, dx,$$

where $f \cdot g = \sum_{s=1}^{2m} f_s \bar{g}_s$, $dx = dx_1 \cdots dx_m$. For $j \in Z^m$, $x \in X$, define $j \cdot x = j_1 x_1 + \cdots + j_m x_m$. Define the linear transformation F: $l^2(S) \to H$ by

$$(Ff)_s(x) = \sum_{j \in Z^m} f_s(j) e^{ij \cdot x}.$$

It is easy to see that F is unitary and that

$$(F^{-1}g)_s(j) = \frac{1}{(2\pi)^m} \int_0^{2\pi} g_s(x) e^{-ij \cdot x} \, dx.$$

Let $\hat{T}_{sr} = \hat{T}_{sr}(x)$ be the $2m \times 2m$ matrix given by

$$T_{sr} = \sum_{j \in I} A(s,j,r) e^{-ij \cdot x}.$$

Now $\hat{T}_{sr}$ corresponds to a linear operator T on H given by

$$(\hat{T}g)_s(x) = \sum_{r=1}^{2m} \hat{T}_{sr} g_r(x).$$

The next theorem shows that T is the transform of the propagator T in H.

Theorem 7: $\hat{T} = FTF^{-1}$.

Proof: It is easy to check that the vectors

$$\{\delta_s e^{ij \cdot x} : j \in Z^m, \ s \in \{1,\ldots,2m\}\},$$

form an orthonormal basis for H. If we show that T and FTF^{-1} agree on these vectors, we are finished. For any $(v,s) = (j,s) \in S$ we have

$$[T\delta_{(v,s)}](v',s')$$
$$= \sum_{(v'',s'')} A[(v',s'),(v'',s'')]\delta_{(v,s)}(v'',s'')$$
$$= A[(v',s'),(v,s)]$$
$$= \sum_{s'',j''} A(s'',j'',s)\delta_{(j-j'',s)}(v',s').$$

Hence,

$$T\delta_{(j,s)} = \sum_{s'',j''} A(s'',j'',s)\delta_{(j-j'',s)}.$$

We therefore obtain

$$FTF^{-1}\delta_s e^{ij\cdot x}$$
$$= FT\delta_{(j,s)} = \sum_{s'',j''} A(s'',j'',s)e^{-ij''\cdot x}\delta_{s''}e^{ij\cdot x}$$
$$= T\delta_s e^{ij\cdot x}. \quad \square$$

Corollary 8: If $q=(j,s)$, $q'=(j',s')$, then

$$A_n(q,q') = \langle \hat{T}^n \delta_s e^{ij\cdot x}, \delta_{s'} e^{ij'\cdot x}\rangle.$$

Instead of finding the nth power (or spectral resolution) of the infinite-dimensional operator T, Corollary 8 reduces the computation of $A_n(q,q')$ to finding the nth power of the $2m\times 2m$ matrix $\hat{T}_{sr}$. The next corollary reduces this computation even further.

Corollary 9: Suppose that the matrix $\hat{T}_{sr}$ has a complete set of unit eigenvectors $\psi_k(x)$ with corresponding eigenvalues $\lambda_k(x)$, $k=1,...,2m$. If $q=(j,s)$, $q'=(j',s')$, we have

$$A_n(q,q') = \frac{1}{(2\pi)^m}\sum_k \int_0^{2\pi} \lambda_k^n \bar{\psi}_{ks}\psi_{ks'} e^{i(j-j')\cdot x}\,dx.$$

Proof: Let P_k be the one-dimensional projection onto ψ_k, $k=1,...,2m$. Applying Corollary 8, we have

$$A_n(q,q') = \left\langle \sum_k \lambda_k^n P_k \delta_s e^{ij\cdot x}, \delta_{s'} e^{ij'\cdot x}\right\rangle$$
$$= \left\langle \sum_k \lambda_k^n (\delta_s e^{ij\cdot x}\cdot\psi_k)\psi_k, \delta_{s'} e^{ij'\cdot x}\right\rangle$$
$$= \sum_k \langle e^{ij\cdot x}\bar{\psi}_{ks}\lambda_k^n \psi_k\cdot\delta_{s'}e^{ij'\cdot x}\rangle$$
$$= \sum_k \frac{1}{(2\pi)^m}\int_0^{2\pi} \bar{\psi}_{ks}(x)e^{ij\cdot x}\lambda_k^n(x) \times \psi_{ks'}(x)e^{-ij'\cdot x}\,dx$$
$$= \frac{1}{(2\pi)^m}\sum_k \int_0^{2\pi} \lambda_k \bar{\psi}_{ks}\psi_{ks'} e^{i(j-j')\cdot x}\,dx. \quad \square$$

We shall apply Corollary 9 in the next section, where we consider one-, two-, and three-dimensional lattices.

We now introduce a notation that will be useful in the sequel. Define the following unit vectors in $\mathbf{R}^m$: $\hat{k}_1=(1,0,0,...,0),...,\hat{k}_m=(0,0,...,0,1)$, $\hat{k}_{m+1}=-\hat{k}_1,...,\hat{k}_{2m}=-\hat{k}_m$. We can then represent the phase space as

$$S=\{(j,k): j\in Z^m,\ k\in\{\hat{k}_1,...,\hat{k}_{2m}\}\}.$$

We now assume that the amplitude function has the following simple form:

$$A((j,k),(j+k',k')) = \begin{cases} a, & \text{if } k'=k,\\ be^{i\theta}, & \text{if } k'=-k,\\ ce^{i\phi}, & \text{if } k'\neq\pm k,\\ 0, & \text{otherwise,}\end{cases} \tag{6}$$

where $a,b,c>0$, $\theta,\phi\in[0,2\pi)$.

Physical motivations can be given for taking A to have this form. First it is clear that A is translation invariant and that $A(q,q')=0$ if $q\perp q'$. Second, since probabilities are independent of a multiplicative phase factor, we can take one of the values of A to be positive; hence, we have the value $a>0$. We shall later add conditions on a,b,c,θ,ϕ so that A satisfies Eq. (1) for an amplitude function. This amplitude function describes the following motion. If a particle is initially at the point (j,k), then it moves in one time step in the "forward direction" to the point $(j+k,k)$ with amplitude a, in the "backward direction" to the point $(j-k,-k)$ with amplitude $be^{i\theta}$, and in the "orthogonal directions" to the points $(j+k',k')$ $k'\neq\pm k$, with amplitude $ce^{i\phi}$. Since there is no physical way to distinguish between the various orthogonal directions, they all have the same amplitude.

We now find conditions on a,b,c,θ,ϕ that are necessary for A to be an amplitude function. Let R_0 be the permutation on the set $\{\hat{k}_1,...,\hat{k}_{2m}\}$ defined by $R_0\hat{k}_j=\hat{k}_{j+1}\pmod{2m}$. For $f\in l^2(S)$, the propagator satisfies

$$(Tf)(j,k) = \sum A((j,k),(j',k'))f(j',k')$$
$$= af(j+k,k) + be^{i\theta}f(j+R_0^m k, R_0^m k)$$
$$+ ce^{i\phi}\sum\{f(j+R_0^r k, R_0^r k):$$
$$r=1,...,2m-1,\ r\neq m\}.$$

Let S and R be the linear operators on $l^2(S)$ defined by $Sf(j,k)=f(j+k,k)$ and $Rf(j,k)=f(j,R_0k)$. It is easy to check that the "translation operator" S is unitary and $S^*f(j,k)=f(j-k,k)$. Moreover, the "rotation operator" R is unitary and $R^*=R^{2m-1}$. We then have

$$T=S\left[aI+be^{i\theta}R^m+ce^{i\phi}\sum\{R^r:\right.$$
$$\left. r=1,...,2m-1,\ r\neq m\}\right].$$

Theorem 10: The propagator T is unitary if and only if the following three equations hold:

(a) $a^2+b^2+2(m-1)c^2=1$;

(b) $ab\cos\theta+(m-1)c^2=0$;

(c) $a\cos\phi+b\cos(\theta-\phi)+(m-2)c=0$, if $m\neq 1$.

Proof: Let

$$L=aI+be^{i\theta}R^m+ce^{i\phi}\sum\{R^r:\ r=1,...,2m-1,\ r\neq m\},$$

so that $T=SL$. Since S is unitary, T is unitary if and only if L is unitary. Now

$$LL^*=\left(aI+be^{i\theta}R^m+ce^{i\phi}\sum_{r\neq m}R^r\right)$$

$$\times\left(aI + be^{-i\theta}R^m + ce^{-i\phi}\sum_{r\neq m} R^r\right)$$
$$= [a^2 + b^2 + 2(m-1)c^2]I$$
$$+ 2[ab\cos\theta + (m-1)c^2]R^m$$
$$+ 2c[a\cos\phi + b\cos(\theta-\phi)$$
$$+ (m-2)c]\sum_{r\neq m} R^r.$$

The result now follows. □

Corollary 11: If A is an amplitude function, then

$$|a + be^{i\theta} + 2(m-1)ce^{i\phi}|^2 = 1.$$

Proof: Applying (a), (b), and (c) of Theorem 10 we obtain

$$|a + be^{i\theta} + 2(m-1)ce^{i\phi}|^2$$
$$= a^2 + b^2 + 4(m-1)^2c^2$$
$$+ 2ab\cos\theta + 4(m-1)c$$
$$\times[a\cos\phi + b\cos(\theta-\phi)]$$
$$= a^2 + b^2 + 4(m-1)^2c^2$$
$$- 2(m-1)c^2 - 4(m-1)(m-2)c^2$$
$$= a^2 + b^2 + 2(m-1)c^2 = 1.$$ □

We interpret Corollary 11 as follows: Let B be the event that the particle is at the nearest neighbor of (j,k) given that it was at (j,k) the previous time step. Then B occurs with certainty. Notice that this is different from the result given by (a), which says the sum of the probabilities that the particle reaches a nearest neighbor in one time step is unity. More generally, we saw in Theorem 1(a) that $\Sigma_q |A_n(q_0,q)|^2 = 1$. However, when A is given by (6) we also have the following.

Corollary 12: If A is an amplitude function, then $|\Sigma_q A_n(q_0,q)|^2 = 1$.

Proof: The expression $\Sigma_q A_n(q_0,q)$ is the sum of the amplitudes of all n-paths with initial point q_0. It easily follows by induction on n that this sum equals $[a + be^{i\theta} + 2(m-1)ce^{i\phi}]^n$. The result now follows from Corollary 11. □

Theorem 10 gives a necessary and sufficient condition for A to be an amplitude function. However, we then only have the three equations (a), (b), and (c) to find the five quantities a,b,c,θ, and ϕ. In order to determine these quantities uniquely, we need two more physically motivated equations. One of these equations can be obtained as follows. Let $0\leqslant v\leqslant 1$ be a parameter. If the particle is massive, v would correspond to the particle's speed (we set the speed of light to unity) or deBroglie frequency, and if the particle is massless (say a photon), v would correspond to the particle's frequency. Suppose the particle is initially at the point $q_0 = (0,\hat{k}_1)$. We assume that after one time step, the particle's average position is v. Let f: $S\to\mathbb{R}$ be the position observable $f((j,k)) = j$. Then

$$v = E_1(f|q_0) = \sum_q f(q)P_1(q_0,q) = a^2 - b^2. \tag{7}$$

There seem to be various choices for a fifth equation depending on our particle model. One approach is given in the following.

Theorem 13: Suppose $m\geqslant 2$ and A is an amplitude function of the form (6). If (7) is satisfied and a has its minimum possible value, then $a = (1+v)/2$ $b = (1-v)/2$, $c = [(1-v)^2/(m-1)]^{1/2}/2$, $\theta = \pi$, and

$$\cos\phi = [(2-m)/2v][(1-v^2)/(m-1)]^{1/2}.$$

Proof: It follows from Theorem 10(b) that $(m-1)c^2\leqslant ab$. Applying Theorem 10(a) and (7) we obtain $(1+v)/2\leqslant a$. Since a has its minimum possible value, $a = (1+v)/2$. The result now follows from Theorem 10(a), (b), (c), and (7). □

Except for the case $m = 2$, the above result is not very satisfactory since the $\cos\phi$ equation requires that $v\geqslant (m-2)/m$. Another approach will be given in the next section.

IV. LOW-DIMENSIONAL LATTICES

In this section we shall consider one-, two-, and three-dimensional infinite lattices. Besides (a), (b), (c) of Theorem 10 and Eq. (7), we shall usually make another physically motivated assumption for the amplitude function. We begin with the one-dimensional case.

Let $V = Z$ be the one-dimensional, infinite linear lattice. In this case, Eq. (6) becomes

$$A((j,k),(j+k',k')) = \begin{cases} a, & \text{if } k' = k, \\ be^{i\theta}, & \text{if } k' \neq k, \\ 0, & \text{otherwise,} \end{cases} \tag{8}$$

where $a,b>0$, $\theta\in[0,2\pi)$. In this case only (a) and (b) of Theorem 10 are applicable. These and (7) give $a^2 + b^2 = 1$, $\cos\theta = 0$, and $a^2 - b^2 = v$, respectively. Therefore, $a = [(1+v)/2]^{1/2}$, $b = [(1-v)/2]^{1/2}$, and we take $\theta = \pi/2$ for definiteness.

We now use the methods developed in Sec. III to find a closed expression for $A_n(q_0,q)$. The matrix elements of $A(s,j,r)$ become

$$A(s,1,r) = \begin{bmatrix} a & 0 \\ ib & 0 \end{bmatrix}, \quad A(s,-1,r) = \begin{bmatrix} 0 & ib \\ 0 & a \end{bmatrix}.$$

Hence, the matrix $\hat{T}_{sr}(x)$ is given by

$$\hat{T}_{sr}(x) = \begin{bmatrix} ae^{-ix} & ibe^{ix} \\ ibe^{-ix} & ae^{ix} \end{bmatrix}.$$

Notice that $\hat{T}_{sr}(x)$ is a unitary matrix. The eigenvalues of $\hat{T}_{sr}(x)$ are $\lambda_1 = a\cos x + i\alpha(x)$, $\lambda_2 = \bar{\lambda}_1$, where $\alpha(x) = (1 - a^2\cos^2 x)^{1/2}$.

The corresponding unit eigenvectors are

$$\psi_1 = N_1(be^{ix}, \alpha(x) + a\sin x),$$
$$\psi_2 = N_2(be^{ix}, -\alpha(x) + a\sin x),$$

where N_1, N_2 are the normalization factors given by

$$N_1^{-2} = 2\alpha(x)[\alpha(x) + a\sin x],$$
$$N_2^{-2} = 2\alpha(x)[\alpha(x) - a\sin x].$$

For $q_0 = (0,\hat{k}_1)$, $q = (j,\hat{k}_1)$ we obtain from Corollary 9 that

$$A_n(q_0,q) = \int_0^{2\pi} e^{ijx}\alpha(x)^{-1}$$
$$\times[\alpha(x)\cos n\phi - ia\sin x\sin n\phi]dx,$$

where

$$\phi = \tan^{-1}[\alpha(x)/a\cos x].$$

For $q_0 = (0,\hat{k}_1)$, $q = (j,\hat{k}_2)$ we obtain

$$A_n(q_0,q) = \int_0^{2\pi} e^{i(j+1)x}\alpha(x)\cos n\phi\, dx,$$

where ϕ is given above.

We next consider the two-dimensional, infinite square lattice $V = Z^2$. We again assume that A is an amplitude function of the form (6) and that (7) holds. If we assume the condition in Theorem 13, we obtain $a = (1+v)/2$, $b = (1-v)/2$, $c = (1-v)^{1/2}/2$, $\theta = \pi$, and $\phi = \pi/2$ or $3\pi/2$.

There is another approach to obtaining reasonable values for A; and this will be important when we get to the three-dimensional case. Consider b as a function $b(v)$ of v. As v increases, more of the particle's motion should be in the forward direction so $b(v)$ should be a decreasing function with $b(1) = 0$. Also when $v = 0$, we require that the motion should be one-dimensional so $b(0) = \sqrt{2}$. The simplest function satisfying these conditions is $b(v) = (1-v)/\sqrt{2}$. We then obtain $a = [(1+v^2)/2]^{1/2}$, $c = [v(1-v)/2]^{1/2}$, $\theta = \cos^{-1}[-v/(1+v^2)^{1/2}]$, $\phi = \tan^{-1}[1 + 2v^2/(1-v)]$.

We now come to the three-dimensional, infinite cubic lattice $V = Z^3$. If we assume the conditions in Theorem 13, we obtain $a = (1+v)/2$, $b = (1-v)/2$, $c = (1-v^2)^{1/2}/2\sqrt{2}$, $\theta = \pi$, $\cos\phi = -(1-v^2)^{1/2}/2\sqrt{2}$. As mentioned earlier, this last equation has a solution if and only if $v \geqslant \frac{1}{3}$. Thus, in this approach small values of v are not admissible.

We therefore use the second approach employed in the two-dimensional case. By that same reasoning, we obtain $a = [(1+v^2)/2]^{1/2}$, $b = (1-v)/\sqrt{2}$, $c = [v(1-v)]^{1/2}/2$, $\theta = \cos^{-1}[-v/(1+v^2)^{1/2}]$. Using (c), we can now solve for ϕ. After some algebraic manipulation we obtain

$$\cos\phi = [-\alpha\gamma + \beta(\alpha^2+\beta^2-\gamma^2)^{1/2}]/(\alpha^2+\beta^2), \tag{9}$$

where $\alpha = (1 - v + 2v^2)$, $\beta = 1 - v$, $\gamma = [v(1-v)(1+v^2)/2]^{1/2}$. We must now convince ourselves that (9) has a solution for every $0 \leqslant v \leqslant 1$. It is easy to show that

$$\beta(\alpha^2+\beta^2-\gamma^2)^{1/2} \geqslant \alpha\gamma.$$

Hence, (9) has a solution if and only if the following inequalities hold:

$$\beta(\alpha^2+\beta^2-\gamma^2)^{1/2} \leqslant \alpha^2+\beta^2+\alpha\gamma, \tag{10}$$

$$\gamma^2 \leqslant \alpha^2+\beta^2. \tag{11}$$

Now (10) is easily verified, and (11) is equivalent to

$$9v^4 - 9v^3 + 13v^2 - 9v + 4 \geqslant 0. \tag{12}$$

Since

$$9v^4 - 9v^3 + 13v^2 - 9v + 4 \geqslant 13v^4 - 9v + 4,$$

Eq. (12) holds if the function $f(v) = 13v^4 - 9v + 4$ is nonnegative or all $0 \leqslant v \leqslant 1$. Now $f(0) = 4$, $f(1) = 8$ and f attains a relative minimum at $v_0^3 = \frac{9}{52}$ or $v_0 = 0.5573$. Since $f(v_0) = 0.2383$ we are finished.

We conclude this section by considering infinite triangular lattices. In the two-dimensional case, the plane is tessellated with equilateral triangles. We define V to be the set of all vertices of these triangles. For $v,v' \in V$, we define $v \perp v'$ if v and v' are vertices of the same triangle. Then each vertex has six nearest neighbors. Assume that A has the form (6), where a corresponds to the forward direction, $be^{i\theta}$ to the backward direction, and $ce^{i\phi}$ to the other four directions. The values of A then reduce to the $V = Z^3$ case. In three dimensions, $\mathbb{R}^3$ is tessellated with regular tetrahedra and each vertex has 12 nearest neighbors. The values of A then reduce to the $V = Z^6$ case.

V. FINITE GRAPHS

While infinite graphs may be useful for describing the motion of a quantum particle in space, finite graphs may be important in the description of "elementary" particles themselves. For example, in the quark model, mesons are composed of a quark and antiquark while baryons are composed of three quarks or three antiquarks. Thus, two- and three-vertex graphs may give a useful description of the hadrons. In other particle models, finite graphs with an even number of vertices can describe bosons and finite graphs with an odd number of vertices can describe fermions. In this section we shall consider only finite graphs of a very simple type.

Let $V = \{v_1,...,v_N\}$ be a finite set with $|V| = N \geqslant 2$. We define $v_j \perp v_j$, if $|j - j'| = 1$ or $N-1$. Denoting the set of edges by E, we obtain an *N-graph* $G_N = (V,E)$. For $N \geqslant 3$, each vertex has precisely two incident edges. We call $\{v_j, v_{j+1}\}, j = 1,...,N$ ($j+1$ is taken mod N) the *forward edge from* v_j and $\{v_j,v_{j-1}\}, j = 1,...,N$ ($j-1$ is taken mod N) the *backward edge from* v_j. In order to include G_2 we assume that G_2 is not a graph but is actually a multigraph with two edges, which we denote v_1v_2 and v_2v_1. Then v_1v_2, v_2v_1 are the forward edges from v_1,v_2, respectively, and v_2v_1, v_1v_2 are the backward edges from v_1,v_2, respectively. The phase space on G_N can be represented as

$$S = \{(j,k): j \in \{1,...,N\},\ k = \pm 1\},$$

where $k = 1(-1)$ corresponds to the forward (backward) edges from v_j.

Let $A: S \times S \to \mathbb{C}$ be an amplitude function of the form (8) (with $j + k'$ taken mod N). It easily follows that $a^2 + b^2 = 1$ and $\theta = \pi/2$ or $3\pi/2$. For definiteness we take $\theta = \pi/2$. If we also assume $a^2 - b^2 = v$ [Eq. (7)] then we obtain $a = [(1+v)/2]^{1/2}$, $b = [(1-v)/2]^{1/2}$. However, this last assumption is not necessary for what we do in the sequel. Now $l^2(S)$ is a $2N$-dimensional Hilbert space with orthonormal basis $\delta_{(j,k)}, j = 1,...,N, k = \pm 1$. The propagator T_N satisfies

$$(T_N f)(j,k) = af(j+k,k) + ibf(j-k,-k).$$

It follows that

$$T_N\delta_{(j,k)} = \alpha\delta_{(j-k,k)} + ib\delta_{(j-k,-k)}. \tag{13}$$

Relative to the basis $\delta_{(j,k)}$, T_N can be represented by a $2N \times 2N$ matrix whose entries are given by (13). Suppose the unitary operator T_N has eigenvalues $\lambda_1,...,\lambda_{2N}$ with corresponding normalized eigenvectors $\psi_1,...,\psi_{2N}$. According to the discussion following Corollary 6, we have

$$A_n(q_0,q) = \sum_r \lambda_r^n \psi_r(q_0)\bar{\psi}_r(q). \tag{14}$$

We first consider G_2. In this case the matrix T_2 becomes

$$T_2 = \begin{bmatrix} 0 & 0 & a & ib \\ 0 & 0 & ib & a \\ a & ib & 0 & 0 \\ ib & a & 0 & 0 \end{bmatrix}.$$

The eigenvalues of T_2 are $\lambda_1 = a + ib$, $\lambda_2 = a - ib$, $\lambda_3 = -\lambda_1$, and $\lambda_4 = -\lambda_2$. The corresponding normalized eigenvectors become

$$\psi_1 = \tfrac{1}{2}(1,1,1,1),$$
$$\psi_2 = \tfrac{1}{2}(1,-1,1,-1),$$
$$\psi_3 = \tfrac{1}{2}(1,1,-1,-1),$$

and

$$\psi_4 = \tfrac{1}{2}(1,-1,-1,1).$$

In functional form we have $\psi_1(j,k) = \frac{1}{2}$, $\psi_2(j,k) = \frac{1}{2}k$, $\psi_3(j,k) = \frac{1}{2}(-1)^{j+1}$, and $\psi_4(j,k) = \frac{1}{2}(-1)^{j+1}k$, with $j = 1,2$, $k = \pm 1$. If $q_0 = (j,k)$ and $q = (j',k')$, then applying (14) gives

$$\begin{aligned} A_n(q_0,q) &= \tfrac{1}{4}[(a+ib)^n + (a-ib)^n kk' \\ &\quad + (-a-ib)^n(-1)^{j+j'} \\ &\quad + (-a+ib)^n(-1)^{j+j'}kk'] \\ &= \tfrac{1}{4}[1+(-1)^{n+j+j'}] \\ &\quad \times [(a+ib)^n + (a-ib)^n kk']. \end{aligned}$$

Letting $\theta = \tan^{-1} b/a$ we obtain

$$A_n(q_0,q) = \begin{cases} \frac{1}{2}[1+(-1)^{n+j+j'}]\cos n\theta, & \text{if } k = k', \\ (i/2)[1+(-1)^{n+j+j'}]\sin n\theta, & \text{if } k \neq k'. \end{cases} \tag{15}$$

It follows from (15) that

$$\begin{aligned} A_n(q_0,j') &= A_n(q_0,(j',1)) + A_n(q_0,(j',-1)) \\ &= \tfrac{1}{2}[1+(-1)^{n+j+j'}]\, e^{in\theta}. \end{aligned}$$

Hence,

$$\begin{aligned} P_n(q_0,j') &= \tfrac{1}{4}|1+(-1)^{n+j+j'}|^2 \\ &= \begin{cases} 1, & \text{if } n+j+j' \text{ is even}, \\ 0, & \text{if } n+j+j' \text{ is odd}. \end{cases} \end{aligned}$$

Now suppose that the particle evolves under the influence of a momentum independent potential $V: S \to \mathbb{R}$. Then V has the form $V((1,k)) = \alpha$, $V((2,k)) = \beta$, $k = \pm 1$. According to Corollary 6, the propagator T_V for the perturbed amplitude A^V satisfies $T_V = e^{-iV}T_2$. We can represent e^{-iV} by the unitary matrix $e^{-iV} = \operatorname{diag}(e^{-i\alpha}, e^{-i\alpha}, e^{-i\beta}, e^{-i\beta})$. The eigenvalues of T_V are $\lambda_1 = (a+ib)e^{-i(\alpha+\beta)/2}$, $\lambda_2 = (a-ib)e^{-i(\alpha+\beta)/2}$, $\lambda_3 = \lambda_1$, and $\lambda_4 = -\lambda_2$. The corresponding normalized eigenvectors become

$$\psi_1 = \tfrac{1}{2}(e^{-i\alpha/2}, e^{-i\alpha/2}, e^{-i\beta/2}, e^{-i\beta/2}),$$
$$\psi_2 = \tfrac{1}{2}(e^{-i\alpha/2}, -e^{-i\alpha/2}, e^{-i\beta/2}, -e^{-i\beta/2}),$$
$$\psi_3 = \tfrac{1}{2}(e^{-i\alpha/2}, e^{-i\alpha/2}, -e^{-i\beta/2}, -e^{-i\beta/2}),$$
$$\psi_4 = \tfrac{1}{2}(e^{-i\alpha/2}, -e^{-i\alpha/2}, -e^{-i\beta/2}, e^{-i\beta/2}).$$

In functional form we have

$$\begin{aligned} \psi_1(j,k) &= \tfrac{1}{2}[e^{-i\alpha/2}(1+(-1)^{j+1}) \\ &\quad + e^{-i\beta/2}(1+(-1)^j)], \\ \psi_2(j,k) &= (k/2)[e^{-i\alpha/2}(1+(-1)^{j+1}) \\ &\quad + e^{-i\beta/2}(1+(-1)^j)], \\ \psi_3(j,k) &= [(-1)^{j+1}/2][e^{-i\alpha/2}(1+(-1)^{j+1}) \\ &\quad + e^{-i\beta/2}(1+(-1)^j)], \\ \psi_4(j,k) &= [(-1)^{j+1}k/2][e^{-i\alpha/2}(1+(-1)^{j+1}) \\ &\quad + e^{-i\beta/2}(1+(-1)^j)]. \end{aligned}$$

The general expression for $A_n^V(q_0,q)$ corresponding to (15) becomes quite complicated and it is simpler to divide it into cases. For the case $q_0 = (1,k)$, $q = (2,k')$, upon applying the analog of (14) we obtain

$$\begin{aligned} &A_n^V(q_0,q) \\ &\quad = \tfrac{1}{4}\exp[-i(n+1)(\alpha+\beta)/2][1-(-1)^n] \\ &\qquad \times [(a+ib)^n + (a-ib)^n kk'] \\ &\quad = \begin{cases} \frac{1}{2}\exp[-i(n+1)(\alpha+\beta)/2][1-(-1)^n] \\ \qquad \times \cos n\theta, & \text{if } k = k', \\ \frac{1}{2}\exp[-i(n+1)(\alpha+\beta)/2][1-(-1)^n] \\ \qquad \times \sin n\theta, & \text{if } k \neq k'. \end{cases} \end{aligned}$$

In particular,

$$\begin{aligned} A_n^V(q_0,2) &= A_n^V(q_0,(2,1)) + A_n^V(q_0,(2,-1)) \\ &= \tfrac{1}{2}\exp[-i(n+1)(\alpha+\beta)/2] \\ &\quad \times [1-(-1)^n]e^{in\theta}, \end{aligned}$$

and

$$P_n^V(q_0,2) = \tfrac{1}{4}|1-(-1)^n|^2 = \begin{cases} 0, & \text{if } n \text{ is even}, \\ 1, & \text{if } n \text{ is odd}. \end{cases}$$

For the case $q_0 = (1,k)$, $q = (1,k')$ we obtain

$$\begin{aligned} &A_n^V(q_0,q) \\ &\quad = \begin{cases} \frac{1}{2}\exp[-i((n+2)\alpha + n\beta)/2][1+(-1)^n] \\ \qquad \times \cos n\theta, & \text{if } k = k', \\ (i/2)\exp[i((n+2)\alpha + n\beta)/2][1+(-1)^n] \\ \qquad \times \sin n\theta, & \text{if } k \neq k'. \end{cases} \end{aligned}$$

In particular,

$$\begin{aligned} &A_n^V(q_0,1) \\ &\quad = \tfrac{1}{2}\exp[-i((n+2)\alpha + n\beta)/2][1+(-1)^n]e^{in\theta} \end{aligned}$$

and

$$P_n^V(q_0,1) = \tfrac{1}{4}|1+(-1)^n|^2 = \begin{cases} 1, & \text{if } n \text{ is even}, \\ 0, & \text{if } n \text{ is odd}. \end{cases}$$

We next consider G_3. The eigenvalues of the unitary 6×6 matrix T_3 are $\lambda_1 = a + ib$, $\lambda_2 = a - ib$, $\lambda_3 = \lambda_4 = [-a + i(4-a^2)^{1/2}]/2$, and $\lambda_5 = \lambda_6 = [-a - i(4-a^2)^{1/2}]/2$. The corresponding normalized eigenvectors become

$$\psi_1 = 6^{-1/2}(1,1,1,1,1,1),$$
$$\psi_2 = 6^{-1/2}(,1,-1,1,-1,1,-1),$$
$$\psi_3 = (4-a^2)^{-1/2}(\lambda_3, -ib, -(\lambda_3 + a), 0, a, ib),$$

$$\psi_4 = (4-a^2)^{-1/2}(0,-(\lambda_4+a),-ib,\lambda_4,ib,a),$$
$$\psi_5 = (4-a^2)^{-1/2}(\lambda_5,-ib,-(\lambda_5+a),0,a,ib),$$
$$\psi_6 = (4-a^2)^{-1/2}(0,-(\lambda_6+a),-ib,\lambda_6,ib,a).$$

We can now compute $A_n(q_0,q)$ using (14). For example, let $q_0=(1.1)$, $q=(j,k)$. Then

$$\begin{aligned} A_n(q_0,q) &= \tfrac{1}{6}[\lambda_1^n\bar{\psi}_1(q)+\lambda_2^n\bar{\psi}_2(q)] \\ &\quad + [1/(4-a^2)][\lambda_3^{n+1}\bar{\psi}_3(q)+\lambda_5^{n+1}\bar{\psi}_5(q)] \\ &= \tfrac{1}{6}[\lambda_1^n + k\bar{\lambda}_1^n] \\ &\quad + [1/(4-a^2)][\lambda_3^{n+1}\bar{\psi}_3(q)+\bar{\lambda}_3^{n+1}\bar{\psi}_5(q)]. \end{aligned}$$

If $k=1$, we have

$$\begin{aligned} A_n(q_0,q) &= \tfrac{1}{6}[\lambda_1^n+\bar{\lambda}_1^n] \\ &\quad + [1/(4-a^2)][\lambda_3^{n+1}\bar{\psi}_3(q)+\bar{\lambda}_3^{n+1}\psi_3(q)] \\ &= \tfrac{1}{3}\,\mathrm{Re}\,\lambda_1^n + [2/(4-a^2)]\mathrm{Re}\,\lambda_3^{n+1}\bar{\psi}_3(q). \end{aligned}$$

If $k=-1$, we have

$$\begin{aligned} A_n(q_0,q) &= \tfrac{1}{6}[\lambda_1^n-\bar{\lambda}_1^n] \\ &\quad + [1/(4-a^2)][\lambda_3^{n+1}\bar{\psi}_3(q)+\bar{\lambda}_3^{n+1}\bar{\psi}_3(q)] \\ &= (i/3)\mathrm{Im}\,\lambda_1^n + [2i/(4-a^2)]\bar{\psi}_3(q)\mathrm{Im}\,\lambda_3^{n+1}. \end{aligned}$$

Finally, let us consider G_4. The eigenvalues of the unitary 8×8 matrix T_4 are $\lambda_1=a+ib$, $\lambda_2=a-ib$, $\lambda_3=-\lambda_1$, $\lambda_4=-\lambda_2$, $\lambda_5=\lambda_6=i$, and $\lambda_7=\lambda_8=-i$. The corresponding normalized eigenvectors become

$$\psi_1 = 8^{-1/2}(1,1,1,1,1,1,1,1),$$
$$\psi_2 = 8^{-1/2}(1,-1,1,-1,1,-1,1,-1),$$
$$\psi_3 = 8^{-1/2}(1,1,-1,-1,1,1,-1,-1),$$
$$\psi_4 = 8^{-1/2}(1,-1,-1,1,1,-1,-1,1),$$
$$\psi_5 = 8^{-1/2}(1,1,ia+b,-ia-b,-1,-1,-ia-b,ia+b),$$
$$\psi_6 = 2^{-1}(1,0,ia,-b,-1,0,-ia,b),$$
$$\psi_7 = 8^{-1/2}(1,1,-ia-b,ia+b,-1-1,ia+b,-ia-b)$$
$$\psi_8 = 2^{-1}(1,0,-ia,b,-1,0,ia,-b).$$

Again, $A_n(q_0,q)$ can be computed using (14).

Continuing in this fashion, one can see similarities in the G_n's for n even (corresponding to bosons) and the G_n's for n odd (corresponding to fermions).

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Transition probability spaces

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Hilbert-space representations of transition probability spaces are studied. The notions of superposition and the superposition principle are introduced. It is shown that, provided the superposition principle and the postulate of minimal superposition are satisfied, transition probability space can be represented by a generalized Hilbert space.

I. INTRODUCTION

In an axiomatic approach to quantum mechanics, Mielnik introduced the concept of transition probability space.[1] The set of all pure states of a quantum-mechanical system is considered as an abstract space with a geometry determined by transition probabilities. In general, the states of a transition probability space need not be realizable in a Hilbert space. Mielnik[1] studied the criteria under which two-dimensional transition probability spaces can be embedded in a Hilbert space. Belinfante[2] studied the structure of three-dimensional transition probability spaces.

In this paper, we study infinite-dimensional transition probability spaces and possibilities of their representations in vector spaces. We show that under only one additional assumption, the so-called "postulate of minimal superposition" introduced by Gudder,[3] a version of the Piron theorem[4] for transition probability spaces can be proved. Cantoni[5] has shown that a transition probability can be obtained on the basis of only the two first Mackey axioms.[6] As a consequence, adding only two additional assumptions to Mackey's first two axioms,[5] a representation of state space in a generalized Hilbert space can be found.

II. BASIC DEFINITIONS AND KNOWN RESULTS

In this section, we introduce the definitions and results of Mielnik[1] and Belinfante.[2]

Let $\mathcal{S}$ be a set of pure states. Denote by $\alpha,\beta,\gamma,\ldots$ the elements of $\mathcal{S}$.

Definition 2.1: A map $T: \mathcal{S}\times\mathcal{S}\to\langle 0,1\rangle$ is called a transition probability if it satisfies

(i) $T(\alpha,\beta)=0$ iff $T(\beta,\alpha)=0$,

(ii) $T(\alpha,\beta)=1$ iff $\alpha=\beta$,

and

(iii) calling α,β orthogonal if

$$T(\alpha,\beta)=T(\beta,\alpha)=0, \quad \sum_{\beta\in R} T(\alpha,\beta)=1$$

for any maximal set R of mutually orthogonal elements of $\mathcal{S}$ and any $\alpha\in\mathcal{S}$.

The sum in Definition 2.1 is thought of as the supremum of all finite partial sums.

A transition probability T is symmetric if

(iv) $T(\alpha,\beta)=T(\beta,\alpha)$, for all $\alpha,\beta\in\mathcal{S}$.

In our considerations, we shall not suppose the symmetry of T. We note that, owing to (i), the orthogonality relation is always symmetric.

A set R of orthogonal elements of $\mathcal{S}$ will be called an orthobase of $\mathcal{S}$ if it satisfies $\Sigma_{\beta\in R}T(\alpha,\beta)=1$ for all $\alpha\in\mathcal{S}$. By (iii), an orthogonal set R is an orthobase iff it is maximal.

Definition 2.2: A set $\mathcal{S}$ with the mapping T satisfying (i)–(iii) of Definition 2.1 is called a transition probability space and denoted by $(\mathcal{S},T)$.

For $A\subset\mathcal{S}$ we denote by $A^{\perp}$ the set of all $\beta\in\mathcal{S}$ that are orthogonal to all elements of A, i.e.,

$$A^{\perp}=\{\beta\in\mathcal{S}: T(\alpha,\beta)=0, \quad \text{for all } \alpha\in A\}.$$

We shall write $A\perp B$, $A,B\subset\mathcal{S}$, if $T(\alpha,\beta)=0$ for any $\alpha\in A$ and $\beta\in B$. If $A=\{\alpha\}$, $B=\{\beta\}$, we write $\alpha\perp\beta$.

Lemma 2.1: Let $A,B\subset\mathcal{S}$. Then

(i) $A\subset B$ implies $B^{\perp}\subset A^{\perp}$,

(ii) $A\subset A^{\perp\perp}=(A^{\perp})^{\perp}$,

(iii) $A\cap A^{\perp}=\emptyset$, $(A\cup A^{\perp})^{\perp}=\emptyset$.

Proof: Straightforward.

Lemma 2.2: For any $\alpha\in\mathcal{S}$, $\{\alpha\}^{\perp\perp}=\{\alpha\}$.

Proof: Let $\{\alpha,\{\beta_i\}_i\}$ be an orthobase of $\mathcal{S}$ (it exists by Zorn's lemma). Then for any $\gamma\in\mathcal{S}$,

$$\sum_i T(\gamma,\beta_i)+T(\gamma,\alpha)=1.$$

If $\gamma\in\{\alpha\}^{\perp\perp}$, then $T(\gamma,\beta_i)=0$ for all i, so that $T(\gamma,\alpha)=1$, which implies that $\gamma=\alpha$.

It is clear that $\mathcal{S}^{\perp\perp}=\mathcal{S}$, i.e., $\emptyset^{\perp}=\mathcal{S}$. Also, $S_1\subset S_2^{\perp\perp}$ implies $S_1^{\perp\perp}\subset S_2^{\perp\perp}$, $S_1S_2\subset\mathcal{S}$. This implies that $S\mapsto S^{\perp\perp}$ is a closure operation.[7] Let $\mathcal{F}(\mathcal{S})=\{S\subset\mathcal{S}: S=S^{\perp\perp}\}$. Then $\mathcal{F}(\mathcal{S})$ is a complete atomistic orthocomplemented lattice with the singleton sets $\{\alpha\}$, $\alpha\in\mathcal{S}$, as the atoms and with the lattice operations defined as follows:

$$\wedge S_i=\cap S_i \quad \text{(the set-theoretical intersection)},$$

$$\vee S_i=(\cup S_i)^{\perp\perp}.$$

Definition 2.3: A subset S of $\mathcal{S}$ is called an orthoclosed subspace of $\mathcal{S}$ if there is a set of mutually orthogonal elements A such that $S=A^{\perp\perp}$.

Lemma 2.3: For any orthogonal set B,

$$B^{\perp\perp}=\left\{\alpha\in\mathcal{S}: \sum_{\beta\in B}T(\alpha,\beta)=1\right\}.$$

Proof: Let α be such that $\Sigma_{\beta\in B}T(\alpha,\beta)=1$ and let γ_0 be such that $T(\beta,\gamma_0)=0$ for all $\beta\in B$ (i.e., $\gamma_0\in B^{\perp}$). Then

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there is $C \subset \mathscr{S}$ such that $B \cup C$ is an orthobase of $\mathscr{S}$ and $\gamma_0 \in C$. We have

$$\sum_{\beta \in B} T(\alpha, \beta) + \sum_{\gamma \in C} T(\alpha, \gamma) = 1,$$

which implies $T(\alpha, \gamma_0) = 0$, i.e., $\alpha \in B^{\perp\perp}$. Now let $\alpha \in B^{\perp\perp}$. Then $\gamma \perp B$ implies $\gamma \perp \alpha$. Let $C \subset \mathscr{S}$ be such that $B \perp C$ and $B \cup C$ is an orthobase of $\mathscr{S}$. Then $T(\alpha, \gamma) = 0$ for all $\gamma \in C$ and

$$\sum_{\beta \in B} T(\alpha, \beta) + \sum_{\gamma \in C} T(\alpha, \gamma) = 1,$$

implies that

$$\sum_{\beta \in B} T(\alpha, \beta) = 1.$$

If $S = B^{\perp\perp}$, where B is an orthogonal set, we shall call B an orthobase of S.

Lemma 2.4: If S is an orthoclosed subspace, then every maximal orthogonal subset of S is an orthobase of S.

Proof: Let $S = B^{\perp\perp}$, where B is an orthobase of S, and let A be any maximal orthogonal subset of S. Then for any $\alpha \in \mathscr{S}$,

$$\sum_{\beta \in B} T(\alpha, \beta) + \sum_{\gamma \in C} T(\alpha, \gamma) = 1,$$

where $C \perp B$ is such that $B \cup C$ is an orthobase of $\mathscr{S}$. If $\alpha \in S^{\perp}$, then $\Sigma_{\gamma \in C} T(\alpha, \gamma) = 1$. By Lemma 2.3, C is an orthobase for S. Now $\gamma \perp C$ implies $\gamma \in S^{\perp\perp} = S$. Therefore, $A \cup C$ is an orthobase of $\mathscr{S}$. If $\alpha \in S$, then $\alpha \perp C$, i.e., $\Sigma_{\beta \in A} T(\alpha, \beta) = 1$. Again by Lemma 2.3, A is an orthobase of S.

If S is an orthoclosed subspace of $\mathscr{S}$, then T restricted to S is a transition probability, i.e., (S,T) is a transition probability space. Let us denote by $\mathscr{O}(\mathscr{S})$ the set of all orthoclosed subspaces of $\mathscr{S}$.

Proposition 2.1: The set $\mathscr{O}(\mathscr{S})$ is an atomistic orthomodular poset.

Proof: From the proof of Lemma 2.4 it follows that $S \in \mathscr{O}(\mathscr{S})$ implies $S^{\perp} \in \mathscr{O}(\mathscr{S})$. Let $S_1, S_2 \in \mathscr{O}(\mathscr{S})$ and let $S_1 \perp S_2$. Let B_1 and B_2 be orthobases of S_1 and S_2, respectively. We have $B_1 \perp B_2$. Further,

$$(B_1 \cup B_2)^{\perp} = B_1^{\perp} \cap B_2^{\perp} = S_1^{\perp} \cap S_2^{\perp} = (S_1 \cup S_2)^{\perp},$$

i.e.,

$$S_1 \vee S_2 = (S_1 \cup S_2)^{\perp\perp} = (B_1 \cup B_2)^{\perp\perp},$$

hence $B_1 \cup B_2$ is an orthobase of $S_1 \vee S_2$. To show orthomodularity, let $A_1, A_2 \in \mathscr{O}(\mathscr{S})$, $A_1 \subset A_2$, and $A_2 \cap A_1^{\perp} = \emptyset$. Let B_1 be an orthobase of A_1. As $\gamma \perp A_1$ iff $\gamma \perp B_1$, there is no $\gamma \in A_2$, $\gamma \perp B_1$. This implies that B_1 is an orthobase of A_2, i.e., $A_1 = A_2$. As by Lemma 2.2, every singleton set $\{\alpha\}$, $\alpha \in \mathscr{S}$, has an orthobase $\{\alpha\}$, and $\mathscr{O}(\mathscr{S})$ is atomistic.

In the preceding propositions we did not need to suppose the symmetry of the transition probability. The following proposition is the only one in which we suppose the symmetry.

Proposition 2.2: If $(\mathscr{S},T)$ is a symmetric transition probability space, then every orthobase of $\mathscr{S}$ has the same cardinality.

Proof: Let B_1 and B_2 be two finite orthobases of $\mathscr{S}$. Owing to the symmetry,

$$\sum_{\beta \in B_2} \sum_{\alpha \in B_1} T(\beta, \alpha) = \sum_{\alpha \in B_1} \sum_{\beta \in B_2} T(\alpha, \beta),$$

which implies that card B_2 = card B_1. Now let B_1 and B_2 be infinite-dimensional orthobases of $\mathscr{S}$. For any $\alpha \in B_1$, $\Sigma_{\beta \in B_2} T(\alpha, \beta) = 1$, so that the set $J(\alpha) = \{\beta \in B_2 : T(\alpha, \beta) \neq 0\}$ is at most countable. Put $A = \cup_{\alpha \in B_1} J(\alpha)$. Then $A \subset B_2$, card B_1 = card $A \leqslant$ card B_2. Similarly we obtain the opposite inequality, i.e., card B_1 = card B_2.

We have $\mathscr{O}(\mathscr{S}) \subset \mathscr{F}(\mathscr{S})$. The following proposition gives us a condition under which every element of $\mathscr{F}(\mathscr{S})$ has an orthobase.

Proposition 2.3: Let there be, for any set P of $\mathscr{O}(\mathscr{S})$ with an at most countable orthobase and any $\alpha \in \mathscr{S}$, $\beta \perp P$ such that $P \vee \{\beta\} \subset P \vee \{\alpha\}$. Then $\mathscr{F}(\mathscr{S}) = \mathscr{O}(\mathscr{S})$.

Proof: Let $S \in \mathscr{F}(\mathscr{S})$ and let B be a maximal orthogonal subset of S. Our aim is to show that $S = B^{\perp\perp}$. Let $\alpha \in S \setminus B^{\perp\perp}$. As $\Sigma_{\beta \in B} T(\alpha, \beta) \leqslant 1$, there is an at most countable subset $B_1 = \{\gamma_1, \gamma_2, \ldots\} \subset B$ such that $T(\alpha, \gamma) = 0$ for any $\gamma \in B \setminus B_1$. By the supposition, there is $\beta \perp B_1$ such that $S \supset B_1^{\perp\perp} \vee \{\alpha\} \supset B_1^{\perp\perp} \vee \{\beta\}$. As $\alpha \perp B \setminus B_1$, $B_1 \perp B \setminus B_1$, and $\beta \in (B_1 \cup \{\alpha\})^{\perp\perp}$, we have $\beta \perp B \setminus B_1$. This implies that $\beta \perp B$, which contradicts the maximality of B.

Definition 2.4: A transition probability space is called irreducible if it cannot be written as a set union of two orthogonal transition probability spaces.

Every transition probability space can be written as a set-theoretical union of mutually orthogonal irreducible transition probability spaces.

III. SUPERPOSITIONS OF STATES AND THE SUPERPOSITION PRINCIPLE

In the sequel, $(\mathscr{S},T)$ is a transition probability space.

Definition 3.1: Let $P \subset \mathscr{S}$. We say that $\alpha \in \mathscr{S}$ is a superposition of P if $T(\gamma, \beta) = 0$ for all $\gamma \in P$ implies $T(\alpha, \beta) = 0$ ($\beta \in \mathscr{S}$).

Denote by $\overline{P}$ the set of all superpositions of P, i.e.,

$$\overline{P} = \{\alpha \in \mathscr{S} : T(\gamma, \beta) = 0 \ \forall \gamma \in P \Rightarrow T(\alpha, \beta) = 0\}.$$

Lemma 3.1: $A^{\perp\perp} = \overline{A}$ for any $A \subset \mathscr{S}$.

Proof: Let $\alpha \in A^{\perp\perp}$, and let $T(\gamma, \beta) = 0$ for all $\gamma \in A$. This implies that $\beta \in A^{\perp}$, i.e., $T(\alpha, \beta) = 0$, hence $\alpha \in \overline{A}$. Let $\alpha \in \overline{A}$. If $\beta \in A^{\perp}$, then $T(\beta, \gamma) = 0$ for all $\gamma \in A$. This implies that $T(\alpha, \beta) = 0$, i.e., $\alpha \in A^{\perp\perp}$.

Definition 3.2: A subset S of $\mathscr{S}$ is called a (linear) subspace if it is closed under the formations of the superpositions of any pair of its elements, i.e., if $\{\alpha, \beta\}^{-} \subset S$ for any $\alpha, \beta \in S$.

If S is not a linear subspace, we denote by $\Lambda(S)$ the smallest linear subspace containing S.

Lemma 3.2: For any $S_1, S_2, S \subset \mathscr{S}$ and $\alpha, \beta \in \mathscr{S}$,

(i) $S \subset \Lambda(S) \subset \overline{S}$,

(ii) $S_1 \subset \Lambda(S_2)$ implies $\Lambda(S_1) \subset \Lambda(S_2)$,

(iii) $\Lambda(S) = \overline{S}$ if $S \in \{\emptyset, \{\alpha\}, \{\alpha, \beta\}\}$.

Proof: Straightforward.

Properties (i) and (ii) of Lemma 3.2 imply that

$S \to \Lambda(S)$ is a closure operation.[7] Let $\mathscr{L}(\mathscr{S}) = \{S \subset \mathscr{S}: S = \Lambda(S)\}$. Then $\mathscr{L}(\mathscr{S})$ is a complete atomistic lattice with the singleton sets $\{\alpha\}, \alpha \in \mathscr{S}$, as the atoms and with the lattice operations $\wedge S_i = \cap S_i$ (set-theoretical intersection) and $\Sigma S_i = \Lambda(\cup S_i)$. We note that Σ is different from $\vee$ in the set $\mathscr{F}(\mathscr{S})$. By Lemma 3.2 (i), $\mathscr{F}(\mathscr{S}) \subset \mathscr{L}(\mathscr{S})$. We shall call the elements of $\mathscr{F}(\mathscr{S})$ closed (linear) subspaces of $\mathscr{S}$. We have

orthoclosed subspaces	$\mathscr{O}(\mathscr{S})$—atomistic orthomodular poset
	$\cap$
closed subspaces	$\mathscr{F}(\mathscr{S})$—atomistic complete ortholattice
	$\cap$
subspaces	$\mathscr{L}(\mathscr{S})$—atomistic complete lattice.

In what follows, we shall suppose that the Gudder's postulate of minimal superposition (MSP) holds in $(\mathscr{S},T)$ (see Ref. 3).

Definition 3.3: Let $S = \{\alpha_1,\alpha_2,...,\alpha_n\}$ be a finite subset of $\mathscr{S}$. We say that α is a minimal superposition of S if $\alpha \in \overline{S}$ and $\alpha \notin \overline{Q}$ for any proper subset Q of S.

Definition 3.4: We say that the postulate of minimal superposition (MSP) holds in $(\mathscr{S},T)$ if for any finite subset S of $\mathscr{S}$ and any minimal superposition α of S the following is satisfied: $(Q_1 \cup \{\alpha\})^- \cap \overline{Q}_2 \neq \emptyset$ for any $Q_1Q_2 \subset S$, $Q_1 \neq \emptyset$, $Q_2 \neq \emptyset$, such that $Q_1 \cup Q_2 = S$ and $Q_1 \cap Q_2 = \emptyset$.

Proposition 3.1: If MSP holds in $(\mathscr{S},T)$, then for any $\alpha,\beta,\gamma \in \mathscr{S}$, mutually different, $\alpha \in \{\beta,\gamma\}^-$ iff $\beta \in \{\alpha,\gamma\}^-$ iff $\gamma \in \{\alpha,\beta\}^-$.

Proof: As α is a minimal superposition of $\{\beta,\gamma\}$, MSP implies that $\{\alpha,\beta\}^- \cap \{\gamma\} \neq \emptyset$, i.e., $\gamma \in \{\alpha,\beta\}^-$.

Definition 3.5: A subset S of $\mathscr{S}$ is independent if for any $\alpha \in S$, $\alpha \notin (S - \{\alpha\})^-$.

Proposition 3.2: Any orthogonal set B in $\mathscr{S}$ is independent.

Proof: Let B be an orthogonal set. Let $\alpha \in (B - \{\alpha\})^- \cap B$. Then for any $\beta \in \mathscr{S}$, $T(\beta,\gamma) = 0$ for all $\gamma \in B - \{\alpha\}$ implies $T(\beta,\alpha) = 0$. But then $T(\alpha,\alpha) = 0$, a contradiction.

If $S = \overline{A}$, and A is independent, we say that A is a base of S. An orthobase is a special case of a base. It is easy to see that a maximal set of independent elements in S, where $S \in \mathscr{F}(\mathscr{S})$, is a base of S.

Proposition 3.3: Let $\{\alpha_1,\alpha_2,...,\alpha_n\}$ and $\{\beta_1,\beta_2,...,\beta_k\}$ be two finite bases of $S \in \mathscr{F}(\mathscr{S})$. If MSP holds, then $n = k$.

The method of the proof is standard, see, e.g., Gudder.[3]

Proposition 3.3 implies that, provided MSP holds, every orthobase of $\mathscr{S}$ has the same cardinality even in a nonsymmetric transition probability space (see Proposition 2.2).

If $S \in \mathscr{F}(\mathscr{S})$ has a finite base $\{\alpha_1,\alpha_2,...,\alpha_n\}$, we call S finite dimensional and put $d(S) = n$. We call $d(S)$ the dimension of S. By Proposition 3.3, $d(S)$ is well defined, provided MSP holds.

Now we shall study the properties of the set $\mathscr{L}(\mathscr{S})$ of linear subspaces of $\mathscr{S}$. We shall suppose that MSP holds in $(\mathscr{S},T)$. As the proofs of the following propositions are the same as the proofs of corresponding statements in the author's previous papers[8] we omit them.

Proposition 3.4: For any finite subset S of $\mathscr{S}$, $\Lambda(S) = \overline{S}$.

We can define independence also in the sense of the operation $S \to \Lambda(S)$: we say that the set A is independent if for any $\alpha \in A$, $\alpha \notin \Lambda(A - \{\alpha\})$. By Proposition 3.4, both definitions of independence are equivalent for finite subsets of $\mathscr{S}$. This implies that, provided MSP holds, every finite-dimensional element of $\mathscr{L}(\mathscr{S})$ belongs to $\mathscr{F}(\mathscr{S})$.

Proposition 3.5: For every $S_1,S_2 \in \mathscr{L}(\mathscr{S})$,

$$S_1 + S_2 \equiv \Lambda(S_1 \cup S_2) = \{\alpha \in \mathscr{S}: \alpha \in \{\beta,\gamma\}^-,\ \beta \in S_1,\ \gamma \in S_2\}.$$

We note that Proposition 3.5 shows us the linear properties of the elements of the set $\mathscr{L}(\mathscr{S})$.

Proposition 3.6: The set $\mathscr{L}(\mathscr{S})$ has the following properties: (i) it is modular; (ii) it has the covering property; (iii) if $\omega \in \mathscr{S}$ and $A \subset \mathscr{S}$ is such that $\omega \in \Lambda(A)$, then there is a finite subset $\{\omega_1,\omega_2,...,\omega_n\} \subset A$ such that $\omega \in \Lambda(\{\omega_1,...,\omega_n\})$; and (iv) to any $S \in \mathscr{L}(\mathscr{S})$ there is $Q \in \mathscr{L}(\mathscr{S})$ such that $S \wedge Q = \emptyset$ and $S + Q = \mathscr{S}$.

For the definitions of modularity and the covering property see, e.g., Maeda and Maeda.[9]

Proposition 3.7: Let $S \in \mathscr{L}(\mathscr{S})$ be finite dimensional. Then $d: Q \to d(Q)$ is a dimension function on $[\emptyset,S] = \{Q \in \mathscr{L}(\mathscr{S}): Q \subseteq S\}$, and $[\emptyset,S]$ is a complemented modular lattice.

Proposition 3.8: For any $S \in \mathscr{F}(\mathscr{S})$ and any finite-dimensional $Q \in \mathscr{F}(\mathscr{S})$, $S \vee Q = S + Q$.

The concept of a superposition enables us to introduce the definition of a superposition principle.[8]

Definition 3.6: We say that a superposition principle (SP) holds in the transition probability space $(\mathscr{S},T)$ if for any $\alpha,\beta \in \mathscr{S}$, $\alpha \neq \beta$, there is $\gamma \in \{\alpha,\beta\}$, $\gamma \neq \alpha$, $\gamma \neq \beta$.

If MSP holds in $(\mathscr{S},T)$, we can define in the set $\mathscr{L}(\mathscr{S})$ the notions of points, lines, and planes: an element S in $\mathscr{L}(\mathscr{S})$ is a point if $d(S) = 1$, it is a line if $d(S) = 2$, and it is a plane if $d(S) = 3$. If α,β are different points, then $\{\alpha,\beta\}^-$ is a line. This yields a new formulation of a superposition principle: a superposition principle holds in $(\mathscr{S},T)$ iff every line in $\mathscr{L}(\mathscr{S})$ contains at least three different points.

To find a connection between the superposition principle and irreducibility, we introduce the notion of a sector.

Definition 3.7: We say that the subspace $S \in \mathscr{L}(\mathscr{S})$ is a sector if

(i) for any $\alpha,\beta \in S$, $\{\alpha,\beta\}^- \neq \{\alpha,\beta\}$,

(ii) for any $\alpha \in S$, $\beta \notin S$, $\{\alpha,\beta\}^- = \{\alpha,\beta\}$.

In the following proposition we do not need the MSP.

Proposition 3.9: If $\mathscr{S} = S_1 \cup S_2$, where $S_1 \perp S_2$, then for every sector S, $S \subset S_1$ or $S \subset S_2$.

Proof: Let S be a sector. Suppose that there are $\alpha,\beta \in S$

such that $\alpha \in S_1, \beta \in S_2$. By the definition of a sector, there is a $\gamma \in \{\alpha,\beta\}^-, \gamma \neq \alpha, \gamma \neq \beta$. But $\gamma \in S_1 \cup S_2$. Suppose $\gamma \in S_1$. We have $T(\delta,\alpha) = T(\delta,\beta) = 0$ imply $T(\delta,\gamma) = 0$ for $\delta \in \mathscr{S}$. For $\delta \in S_1$ we have $T(\delta,\beta) = 0$, so that $T(\delta,\alpha) = 0$ implies $T(\delta,\gamma) = 0$. This together with $S_2 \perp \alpha$ and $S_2 \perp \gamma$ gives us $\{\alpha\}^\perp \subset \{\gamma\}^\perp$, i.e., $\{\gamma\}^{\perp\perp} \subset \{\alpha\}^{\perp\perp}$ and, by Lemma 2.2, $\gamma = \alpha$. Similarly, if $\gamma \in S_2$, then $\gamma = \beta$, a contradiction.

Proposition 3.9 gives us the following corollary.

Corollary 3.1: If the superposition principle holds in $(\mathscr{S},T)$, then $\mathscr{S}$ is irreducible.

Definition 3.8: We shall say that $\alpha, \beta \in \mathscr{S}$ are perspective if $\alpha = \beta$ or if $\{\alpha,\beta\}^- \neq \{\alpha,\beta\}$. We shall write $\alpha \sim \beta$.

By Definition 3.8, perspectivity is a reflexive and symmetric relation.

Proposition 3.10: If MSP holds, perspectivity is transitive.

Proof: Suppose $\alpha \sim \beta, \beta \sim \gamma$, where α, β, γ are mutually different. If $\gamma \in \{\alpha,\beta\}^-$, then $\beta \in \{\alpha,\gamma\}^-$, and we are finished. Let $\gamma \notin \{\alpha,\beta\}^-$. Then α, β, γ are independent. Let $\delta_1 \in \{\alpha,\beta\}^- - \{\alpha,\beta\}$, $\delta_2 \in \{\beta,\gamma\}^- - \{\beta,\gamma\}$. This implies that $\beta \in \{\gamma,\delta_2\}^-$, hence $\delta_1 \in \{\alpha,\gamma,\delta_2\}^-$. If $\delta_1 \in \{\alpha,\gamma\}^-$, we are finished. If $\delta_1 \in \{\alpha,\delta_2\}^-$, then $\delta_1 \in \{\alpha,\delta_2\}^- \cap \{\alpha,\beta\}^- = \{\alpha\}$, i.e., $\delta_1 = \alpha$, a contradiction. Similarly, $\delta_1 \in \{\gamma,\delta_2\}^-$ implies $\delta_2 \in \{\delta_1,\gamma\}^- \cap \{\beta,\gamma\}^- = \{\gamma\}$. Hence, δ_1 is a minimal superposition. By MSP, $\{\delta_1,\delta_2\}^- \cap \{\alpha,\gamma\}^- \neq \emptyset$, which implies $\{\alpha,\gamma\}^- \neq \{\alpha,\gamma\}$.

Proposition 3.11: Let MSP hold. Then any two different equivalence classes by the perspectivity are mutually orthogonal orthoclosed subspaces.

Proof: Let S_1 and S_2 be two different equivalence classes by perspectivity. Let $\alpha \in S_1$, $\beta \in S_2$. We have $\{\alpha,\beta\}^- = \{\alpha,\beta\}$. By Proposition 3.8, $\{\beta\} + \{\beta\}^\perp = \{\beta\} \vee \{\beta\}^\perp = \mathscr{S}$. If $\alpha \notin \{\beta\}^\perp$, then by Proposition 3.5, $\alpha \in \{\beta,\delta\}^-$ for a $\delta \in \{\beta\}^\perp$. Then $\delta \in \{\alpha,\beta\}^-$, $\delta \neq \alpha, \beta$, a contradiction. Therefore $S_1 \perp S_2$. Now $\mathscr{S} = \cup S_i$, where the S_i are equivalence classes, Let B be an orthobase of $\mathscr{S}$. Clearly, $\alpha \in S_j$ if and only if

$$1 = \sum_{\beta \in B} T(\alpha,\beta) = \sum_i \sum_{\beta \in B \cap S_i} T(\alpha,\beta)$$

$$= \sum_{\beta \in B \cap S_j} T(\alpha,\beta),$$

and, by Lemma 2.3, $B \cap S_j$ is an orthobase for S_j.

Proposition 3.11 implies that every equivalence class by the perspectivity relation is a sector. The following statements are immediate consequences.

Corollary 3.2: If MSP holds in $(\mathscr{S},T)$, then $\mathscr{S}$ can be written as the set-theoretical union of sectors.

Corollary 3.3: If MSP holds, then $(\mathscr{S},T)$ is irreducible if and only if SP holds.

Proposition 3.12: If MSP holds, then every finite-dimensional element of $\mathscr{L}(\mathscr{S})$ has an orthobase.

Proof: Let $S \in \mathscr{L}(\mathscr{S})$ be finite dimensional. Let B be a maximal orthogonal set in S. Put $P = \overline{B} \subset S$. We have $P + P^\perp = \mathscr{S}$, so that for any $\alpha \in S$ there are $\gamma \in P, \beta \in P^\perp$ such that $\alpha \in \{\gamma,\beta\}^-$. By MSP, $\beta \in \{\alpha,\gamma\}^- \subset S$, i.e., $\beta \in P^\perp \wedge S$. This shows that $S = P \vee (P^\perp \wedge S)$. As B is a maximal orthogonal subset of S, $P^\perp \wedge S = \emptyset$, i.e., $S = P$.

A condition for orthomodularity of $\mathscr{F}(\mathscr{S})$ is given in Proposition 2.3. The following statement gives us another necessary and sufficient condition.

Proposition 3.13: If MSP holds, then $\mathscr{F}(\mathscr{S})$ is orthomodular iff for any $S \in \mathscr{O}(\mathscr{S})$ and any $\alpha \in \mathscr{S}$, $S + \{\alpha\} \in \mathscr{O}(\mathscr{S})$.

Proof: If $\mathscr{F}(\mathscr{S})$ is orthomodular, then every $S \in \mathscr{F}(\mathscr{S})$ has an orthobase, i.e., $S + \{\alpha\} \in \mathscr{O}(\mathscr{S})$. On the other hand, let $S + \{\alpha\} \in \mathscr{O}(\mathscr{S})$ for any $S \in \mathscr{O}(\mathscr{S})$ and any $\alpha \in \mathscr{S}$. By orthomodularity, $S + \{\alpha\} = S \vee \{\alpha\} = S \vee (S \vee \{\alpha\}) \wedge S^\perp$. If $\alpha \notin S$, then $(S \vee \{\alpha\}) \wedge S^\perp \neq \emptyset$, so that there is $\beta \in (S \vee \{\alpha\}) \wedge S^\perp$. But then the condition of Proposition 2.3 is fulfilled, so that $\mathscr{O}(\mathscr{S}) = \mathscr{F}(\mathscr{S})$.

IV. REPRESENTATION THEOREMS

For the definitions and theorems used in this section see Baer,[10] Maeda and Maeda,[9] Piron,[4] and Varadarajan.[11]

A theorem of Baer[10] and Proposition 3.6 imply the following statement.

Theorem 4.1: Let $(\mathscr{S},T)$ be a transition probability space such that SP and MSP hold and let there be at least four independent states in $\mathscr{S}$. Then there exists a division ring $\mathscr{K}$ and a vector space $\mathscr{V}$ over $\mathscr{K}$, such that the lattice $\mathscr{L}(\mathscr{S})$ is isomorphic to the lattice $\mathscr{L}(\mathscr{V})$ of all linear subspaces of $\mathscr{V}$.

Theorem 4.1, Propositions 3.4 and 3.8, and Lemma 7.2 and Theorem 7.40 in Varadarajan[11] imply the following theorem.

Theorem 4.2: Let $(\mathscr{S},T)$ be a transition probability space such that SP and MSP hold and let there be at least four independent states in $\mathscr{S}$. Then there exists a division ring $\mathscr{K}$, a vector space $\mathscr{V}$ over $\mathscr{K}$, an involutive antiautomorphism θ of $\mathscr{K}$, and a definite symmetric θ-bilinear form f on $\mathscr{V} \times \mathscr{V}$ such that the set $\mathscr{F}(\mathscr{S})$ is isomorphic to the set $\mathscr{L}_f(\mathscr{V})$ of all f-closed subspaces of $\mathscr{V}$.

Theorem 4.2 yields a version of the Piron theorem for transition probability spaces. The ortholattice $\mathscr{F}(\mathscr{S})$ need not be orthomodular; it is orthomodular iff $\mathscr{F}(\mathscr{S}) \equiv \mathscr{O}(\mathscr{S})$. Owing to the isomorphism of $\mathscr{F}(\mathscr{S})$ and $\mathscr{L}_f(\mathscr{V})$, $\mathscr{F}(\mathscr{S})$ is orthomodular iff $\mathscr{L}_f(\mathscr{V})$ has the Hilbertian property: $M + M^\perp = \mathscr{V}$ for any $M \in \mathscr{L}_f(\mathscr{V})$.

The relation between the transition probability T and the bilinear form f is, in general, not clear; we only know that they both define the orthocomplementation. If the division ring $\mathscr{K}$ is the field of complex numbers $\mathscr{C}$, then, using the Gleason theorem, the following result can be obtained.

Theorem 4.3: Let $(\mathscr{S},T)$ be a transition probability space such that the conditions of Theorem 4.2 are satisifed and let the representing space, which exists by Theorem 4.2, be a complex inner product space $\mathscr{H}$ with the inner product $(\ ,\ )$. Let φ: $\mathscr{F}(\mathscr{S}) \to \mathscr{L}_{(\ ,\ )}(\mathscr{H})$ be the isomorphism stated by Theorem 4.2. Then $T(\alpha,\beta) = \mathrm{tr}(P_{\varphi\{\alpha\}} P_{\varphi\{\beta\}})$ for every $\alpha, \beta \in \mathscr{S}$, where $P_{\varphi\{\alpha\}}, P_{\varphi\{\beta\}}$ are projectors corresponding to subspaces $\varphi\{\alpha\}, \varphi\{\beta\}$ of $\mathscr{L}_{(\ ,\ )}(\mathscr{H})$, respectively. In addition, the space $\mathscr{H}$ is complete.

Proof: Every $\{\alpha,\beta\}$ is contained in some four-dimensional subspace S. The interval $[\emptyset,S]$ with the relative

orthocomplementation is an orthomodular lattice (Proposition 3.12). For any $\alpha \in \mathscr{S}$ and $A \in \mathscr{O}(\mathscr{S})$, put $T_\alpha(A) = \Sigma_{\beta \in B} T(\alpha, \beta)$ where B is an orthobase of A. It is easy to check that T_α is well defined, and it is a probability measure on $\mathscr{O}(\mathscr{S})$. For $\alpha \in S$, the restriction of T_α to $[\emptyset, S]$ is a probability measure on $[\emptyset, S]$. Put $\mu_\alpha(P) = T_\alpha(\varphi^{-1}(P))$, $P \in \varphi(S)$, $\alpha \in S$. Then μ_α is a probability measure on $\varphi(S)$. By the Gleason theorem, there is a trace-class operator D on $\varphi(S)$ such that $\mu_\alpha(P) = \mathrm{tr}(DP)$, $P \in \varphi(S)$. Let $u \in \varphi\{\alpha\}$ be the unit vector and P_u be its corresponding projector. As $\mu_\alpha(P_u) = T_\alpha(\alpha) = 1$, $D = P_u$. Let $\beta \in S, \varphi\{\beta\} = \mathscr{C}v$. Then $T(\alpha, \beta) = T_\alpha(\beta) = \mu_\alpha(P_v) = \mathrm{tr}\, P_u P_v = |(u,v)|^2$. By (iii) of Definition 2.1, Parseval's equality holds for any maximal orthogonal system, so that by Ref. 12, $\mathscr{H}$ is complete.

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Mobility and measurements in nonlinear wave mechanics

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The theory based on the nonlinear Schrödinger equation with an additional term $\lambda(\bar{\psi}\psi)^{\alpha}\psi$ is investigated. The standard quantum mechanical interpretation of ψ is assumed at the beginning of the considerations. It turns out that every finite set of pure states can be transformed with the aid of an adequate time sequence of external potentials into a set of pairwise nearly orthogonal states. As a consequence, there exist measurements more selective than quantum ones. In particular, it is possible to discriminate between various mixtures of states that are equivalent in quantum mechanics. The possibility of existence of deterministic measurements is also discussed.

I. INTRODUCTION

Quantum mechanics is the only linear theory that attempts to describe physical reality completely. However, the rest of physics tells us that linear equations are usually an approximation to a more adequate theory. One can doubt whether the linearity of quantum dynamics is "the law of nature." Yet all the experimental data received up to now supply unequivocal arguments for standard theory. On the other hand, the problem of its interpretation is still open. It may be interesting to check which of the controversial quantum properties depend on the linearity of dynamics. How would the world of quantum waves evolving nonlinearly look?

To answer this question we have to make some elementary assumptions. The systematic developing of physical theory in terms of primitive operations on the system, which can be (at least in principal) performed by an experimenter, has been presented by Lamb,[1] Lubkin,[2] and Mielnik.[3,4] Mielnik has also noted the usefulness of such an approach to the study of nonlinear generalizations of quantum mechanics. Its advantage is the small number of assumptions on observational properties of the system. We have to postulate the set of pure states, the law of evolution in all the admissible external forces and describe results of elementary measurements as functionals on states.

Let the set $\mathscr{P}$ of pure states be essentially the same as in standard quantum mechanics, i.e., the unit sphere in $PL^2(\mathbf{R})$ (projective Hilbert space) or a set dense in it. However, let the Schrödinger equation be modified by a nonlinear term $f(\bar{\psi}\psi)$ (see Ref. 5)

$$i\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial q^2} + v\psi + f(\bar{\psi}\psi)\psi. \tag{1}$$

Here $v = v(q,t)$ are external potentials. As no counterexamples are known in the nonrelativistic theory, we shall assume that all the functions $v(q,t)$, for which there exist global solutions of (1), are allowed as physical potentials. The class of these potentials will be denoted by $\mathscr{V}$. In particular, assume that $\mathscr{V}$ contains potentials changing abruptly with time. Then, the evolution transformations $S(t,v)$, $t\geqslant 0$, $v\in\mathscr{V}$ form a semigroup $\mathscr{D}$ called the mobility semigroup.[2,3] The elements of $\mathscr{D}$ represent all the admissible dynamic transformations of the system the experimenter can cause with the use of external forces.

The last element we need is a primitive interpretation of wave functions. It will be the same as in the linear theory: the elementary measurements consist of the determination of the probability that a particle is "caught" in the space volume Δ. The mathematical description of this probability is given by the functional $\psi\to\int\bar{\psi}(q)E_{\Delta}(q)\psi(q)dq$, where E_{Δ} is the characteristic function of Δ. Such measurements, in which only two outcomes are possible: "yes" or "no," have been called counters (likewise the functionals describing probability of "yes" outcomes).[3] We denote the set of counters by $\mathscr{C}$. It can be constructed out of the set $\mathscr{C}_e$ of elementary counters and the mobility semigroup $\mathscr{D}$. Indeed, before any elementary measurement F, the system can evolve in a certain external field.[2,3] If its evolution is $S\in\mathscr{D}$, then the corresponding functional will be given by $F\cdot S$. Thus, the elements of $\mathscr{C}_e\cdot\mathscr{D}$ represent admissible counters. Moreover, counters can be mixed as well as states.[2,6] In what follows, $\mathscr{C}$ is defined as the convex set spanned by $\mathscr{C}_e\cdot\mathscr{D}$. For mathematical and physical reasons the closure of $\mathscr{C}$ in an adequate topology may be taken.[6]

In quantum mechanics the dynamic transformations are linear and elementary measurements are described by quadratic forms. Therefore only quadratic forms can be interpreted as counters or observables. This yields the peculiar properties of quantum systems called "impossibility principles."[3]

(1) There are different mixtures of pure states that cannot be distinguished by any measurements. The class of such mixtures, the mixed state, is described by the density operator.

(2) The counters registering every system in the state ψ have to register the systems in the state φ with probability $|(\psi|\varphi)|^2$. So called "transition probabilities" are nonzero for nonorthogonal vectors.

The nonlinear modification of evolution (1) changes $\mathscr{D}$ and what follows, the sets of counters and observables. These changes turn out to be radical. Haag and Banier have studied the dynamics with the nonlinear term $\mathbf{A}\cdot\nabla S$, where $\mathbf{A}$ is an external vector potential and S is the phase of wave function. They have proved that every two finite mixtures of pure states are distinguishable.[7] Mielnik has considered finite difference approximations of Eq. (1) for various types of nonlinearities.[4] He has shown that both impossibility principles cease to hold. This has been confirmed in the case of differen-

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tial equations for two nonlinearities: $|\psi|^2\psi$ and $(\ln|\psi|^2)\psi$ (see Ref. 8). The striking example is given by $(\hbar^2\nabla^2\psi)\psi/2m|\psi|$, which leads to classical mechanics.[9]

Below we shall study Eq. (1) with the nonlinear term

$$f(\bar{\psi}\psi)=\lambda(\bar{\psi}\psi)^{\alpha},\quad \lambda\neq 0,\quad \alpha>0,\quad \alpha\neq 2. \tag{2}$$

At first it is shown that $\mathscr{D}$ contains all the unitary operators and the nonlinear one-parameter semigroup generated by the pure nonlinear term in (1) (Sec. II). Then, a transformation of an arbitrary finite set of pure states into a set of pairwise nearly orthogonal states is obtained. This leads to the rejection of both impossibility principles (Sec. III). The considered nonlinear models are "intrinsically classical,"[4] contrary to quantum mechanics, and the problem of their deterministic interpretation arises. We point out that its complete solution depends on the structure of extremal points of $\mathscr{C}$, which has not been found yet (Sec. IV).

II. MOBILITY

To prove various identities we put Schrödinger dynamics into the canonical formalism.[10,11] The nonlinear Schrödinger equation and its conjugate equation can be considered as a pair of canonical equations

$$\begin{aligned}\frac{\partial\psi}{\partial t}q,t&=\frac{\delta H}{\delta\bar{\psi}(q,t)}=\{\psi(q,t),H\},\\ \frac{\partial\bar{\psi}}{\partial t}q,t&=-\frac{\delta H}{\delta\psi(q,t)}=\{\bar{\psi}(q,t),H\},\end{aligned} \tag{3}$$

where functional derivatives are taken of the functional Hamiltonian

$$H=K+V+N, \tag{4}$$

with

$$\begin{aligned}K(\bar{\psi},\psi)&=\frac{1}{2}i\int\bar{\psi}\frac{d^2}{dq^2}\psi\,dq,\\ V(\bar{\psi},\psi)&=-i\int\bar{\psi}v\psi\,dq,\\ N(\bar{\psi},\psi)&=-i\int\tilde{f}(\bar{\psi}\psi)dq.\end{aligned} \tag{5}$$

Here $\tilde{f}$ is a prime function of f: $\tilde{f}'(x)=f(x)$. The Poisson bracket of $F(\bar{\psi},\psi)$ and $G(\bar{\psi},\psi)$ is defined as follows: $\{F,G\}(\bar{\psi},\psi)$

$$=\int\left(\frac{\delta F}{\delta\psi(q,t)}\frac{\delta G}{\delta\bar{\psi}(q,t)}-\frac{\delta F}{\delta\bar{\psi}(q,t)}\frac{\delta G}{\delta\psi(q,t)}\right)dq. \tag{6}$$

Let us denote by S_F^t the one-parameter group generated by F. We shall prove the following theorem.

Proposition 1: Let f be given by (2). Then $\mathscr{D}$ contains all the unitary operators and the nonlinear semigroup S_N^c, $c\geqslant 0$.

Proof: Every canonical evolution can be described as a series of multiple Poisson brackets

$$\psi(t)=\psi+\{\psi,tH\}+\tfrac{1}{2}\{\{\psi,tH\},tH\}+\cdots. \tag{7}$$

Thus S_H^t is determined by the term tH. For $H(t)=K+(a/t)V+N$, we obtain $tH(t)\to aV$ as $t\to 0$. This yields that "shock transformations" S_V^a, $a\in\mathbb{R}$ are contained in $\mathscr{D}$. The S_V^a are unitary operators $\exp\{-iav\}$.[1,2,8,12,13]

Similarly, the following identity holds:

$$S_V^a S_H^t S_V^{-a}=S_{\tilde{H}}, \tag{8}$$

where

$$\tilde{H}=H+a\{H,V\}+(a^2/2)\{\{H,V\},V\}+\cdots. \tag{9}$$

Now, putting in (9) $v(q)=q^2/2$ and

$$H=H_0+(a^2/2)V,\quad H_0=K+N,$$

we obtain by (8) $S_{H_0+aA}^t$, where

$$A=\frac{i}{2}\int\bar{\psi}\left(\frac{d}{dq}q+q\frac{d}{dq}\right)\psi\,dq.$$

In the limit $t\to 0$ with $a=b/t$, $S_{H_0+aA}^t$ tends to S_A^b, $b\in\mathbb{R}$. The dilatation transformations S_A^b are unitary operators that act on wave functions as follows[8,14]:

$$(S_A^b\psi)(q)=e^{b/2}\psi(e^b q). \tag{10}$$

Let us now consider the one-parameter group $t\to S_A^b S_{H_0}^t S_A^{-b}$. Its generator has the following form:

$$\frac{\partial\psi}{\partial t}=e^{-2b}\frac{i}{2}\frac{\partial^2}{\partial q^2}\psi-i\lambda e^{-b\alpha}(\bar{\psi}\psi)^{\alpha}\psi. \tag{11}$$

Therefore this group is generated by the Hamiltonian $H(b)=e^{-2b}K+e^{-b\alpha}N$. If $\alpha\neq 2$, then H_0 is "dynamically decomposable" in two independent generators K and N, namely, let $t=ce^{2b}$. For $\alpha<2$ in the limit $b\to-\infty$, we obtain S_K^c, $c\geqslant 0$. For $\alpha>2$ these transformations can be obtained in the limit $b\to+\infty$. Similarly, S_N^c, $c\geqslant 0$, can be achieved if we let $t=ce^{b\alpha}$ and take the limit $b\to+\infty$ for $\alpha<2$ and $b\to-\infty$ for $\alpha>2$. At the end, the semigroup spanned by S_K^c, $c\geqslant 0$, and S_V^b, $b\in\mathbb{R}$, $v\in\mathscr{V}$, contains all the unitary operators.[12,14] ■

III. MEASUREMENTS, TRANSITION PROBABILITIES, AND MIXED STATES

For every two quantum waves ψ and φ, there is a dynamic unitary transformation $U\in\mathscr{D}$ such that $U\psi=\varphi$ (see Ref. 1). Thus, in the linear theory $\mathscr{D}$ is a transitive on $\mathscr{P}$. Let us consider now transformations of finite sets of (pure) states, i.e., transformations of points in finite Cartesian products of $\mathscr{P}$. The set of transformations on $\mathscr{P}$ transitive on $\times_M^{k=1}\mathscr{P}$ is called M-transitive.[15] It is easily seen that in the linear case $\mathscr{D}$ is not two-transitive, for scalar products have to be conserved. In contrast, the investigations of the particular nonlinear models have shown that their mobility semigroups are two-transitive.[4,8] Here we shall prove the following proposition.

Proposition 2: Let f be given by (2). Then for every $\epsilon>0$ and any M different vectors $(\psi_1,\ldots,\psi_M)$, $M<\infty$, there is an $S\in\mathscr{D}$ such that $|(S\psi_k|S\psi_j)|<\epsilon$ if $k\neq j$.

Proof: The set of wave functions $\psi_1,\ldots,\psi_M$ can be embedded into a K-dimensional subspace, $K\leqslant M$. If M is finite then there is an orthonormal base $(\varphi_1,\ldots,\varphi_K)$ such that for every k the absolute values of coefficients a_{jk}, $1\leqslant j\leqslant M$, in decompositions

$$\psi_j=\sum_{k=1}^{K}a_{jk}\varphi_k$$

are different numbers. The semigroup $\mathscr{D}$ contains a unitary

operator U that transforms $(\varphi_1,...,\varphi_K)$ onto $(\kappa_1,...,\kappa_K)$ (Proposition 1), where

$$\kappa_k = \begin{cases} A(q-k+1)^{1/2\alpha}, & \text{for } q\in(k-1,k), \\ 0, & \text{for } q\notin(k-1,k), \end{cases} \tag{12}$$

where A is a normalization constant independent of k. Thus,

$$U\psi_j = \chi_j = \sum_{k=1}^{K} a_{jk}\kappa_k.$$

Now, $\mathscr{D}$ contains also the nonlinear semigroup S_N^c, $c\geqslant 0$ (Proposition 1)

$$S_N^c(\chi)(q) = \exp\{-ic\lambda\,|\chi|^{2\alpha}(q)\}\chi(q). \tag{13}$$

The scalar products $(S_N^c(\chi_j)|S_N^c(\chi_l))$ depend on c as follows:

$$(S_N^c(\chi_j)|S_N^c(\chi_l)) = \sum_{k=1}^{K} \bar{a}_{jk}a_{lk}\,g_{jlk}(c), \tag{14}$$

where

$$g_{jlk}(c) = \int |\chi_k|^2(q)\exp\{-ic\lambda\,|A|^{2\alpha} \times(|a_{jk}|^{2\alpha} - |a_{lk}|^{2\alpha})(q-k+1)\}dq \tag{15}$$

are (up to a multiplicative constant) Fourier transformations of $|\kappa_k|^2(q)$. Therefore $g_{jlk}(c)\to 0$ if $c\to\infty$ (Riemann–Lebesque lemma). In what follows $(S_N^c(\chi_j)|S_N^c(\chi_k))\to 0$ if $c\to\infty$. ■

Proposition 2 shows operational consequences of generalized Schrödinger dynamics. In particular, it implies the possibility of "selective measurements." Namely, for two finite and disjoint sets of pure states there is always a counter such that positive outcome of the measurement is almost certain for every state of the first set and almost impossible for every state of the second set.

Proposition 3: Let f be given by (2), $(\psi_1,...,\psi_M)$ and $(\varphi_1,...,\varphi_L)$ be finite and disjoint sets of pure states, and $\Delta\subset\mathbb{R}$. For every $\epsilon>0$ there is an $S\in\mathscr{D}$ such that

$$(S(\psi_m)|E_\Delta S(\psi_m))>1-\epsilon,\quad m=1,...,M,$$

and

$$(S(\varphi_1)|E_\Delta S(\varphi_1))<\epsilon,\quad l=1,...,L.$$

Proof: The set $(\psi_1,...,\psi_M,\varphi_1,...,\varphi_L)$ can be transformed by $S_1\in\mathscr{D}$ onto the set of pairwise nearly orthogonal states (Proposition 2). Then, let us take a unitary operator $U_1\in\mathscr{D}$ (Proposition 1), which transforms $(S_1\psi_1,...,S_1\psi_M)$ almost into $E_\Delta L^2(\mathbb{R})$ and $(S_1\varphi_1,...,S_1\varphi_L)$ almost into $(I-E_\Delta)L^2(\mathbb{R})$. Thus, $S=U_1S_1$. ■

As a result, the second impossibility principle of quantum mechanics has to be abandoned. The same thing also concerns the first one. Now, two different finite mixtures of pure states are always distinguishable, for one can construct a counter reacting with various probabilities on systems in these two mixed states.

Proposition 4: Let f be given by (2) and

$$s_1 = \sum_{m=1}^{M} \alpha_m\delta(\psi_m),\quad s_2 = \sum_{l=1}^{L} \beta_l\delta(\varphi_l)$$

be different mixtures of pure states. Then, there is an $F\in\mathscr{C}$ such that $F(s_1)\neq F(s_2)$.

Proof: Let $(\chi_1,...,\chi_K)$, $K\leqslant M+L$, be the set of different pure states that participate in at least one of the mixtures s_1 and s_2. Then, these mixtures can be described as

$$s_1 = \sum_{k=1}^{K} \mu_k\delta(\chi_k),\quad s_2 = \sum_{k=1}^{K} \nu_k\delta(\chi_k),$$

where some of μ_k,ν_k may be equal to zero. There is a χ_j such that $\mu_j\neq\nu_j$, for s_1 and s_2 are different mixtures and there is an $F\in\mathscr{C}$ such that $F(\chi_j)\approx 1$ and $F(\chi_k)\approx 0$ if $k\neq j$ (Proposition 3). This yields $F(s_1)\approx\mu_j\neq\nu_j\approx F(s_2)$. ■

Thus, the set of mixed states is a generalized simplex.[3,4,7,8]

IV. PROBLEM OF DETERMINISTIC INTERPRETATION

The considered models of nonlinear wave mechanics are much more "classical" than quantum mechanics. Does this mean that they are deterministic? To answer, one has to define accurately the term "deterministic." It should mean, first of all, the existence of measurements fully deterministic when applied to the system in a pure state: their outcome should be always "yes" or always "no." Moreover, there should be sufficiently many deterministic counters: every indeterministic counter should be a mixed counter. This means that extreme points of $\mathscr{C}$ should be characteristic functionals of subsets of $\mathscr{P}$ and all such functionals should be counters.

Thus, the question of deterministic interpretation requires the complete description of $\mathscr{C}$. Here we have made a first step toward it. The pure counters may turn out deterministic or not. There are three possibilities.

(1) Pure counters are not deterministic; the theory is intrinsically probabilistic.

(2) There are as well deterministic as indeterministic pure counters; the theory has a "middle of the way" character.

(3) All the pure counters are deterministic; the theory is intrinsically deterministic.

The ultimate answer depends on $\mathscr{D}$ and the choice of $\mathscr{C}_e$. Maybe the theory with primitive Born interpretation will turn out to be of type (1) or (2). Even then, one can hope to construct such elementary counters, which allow one to enlarge $\mathscr{C}$ and make the theory deterministic. Thus, to preserve indeterministic properties, one would have to introduce an impossibility principle, e.g., "it is impossible to construct any elementary counter that is not described by a quadratic form."

The third possibility seems to be especially interesting and promising.[16] Is there a theory that is able to approximate quantum mechanics with arbitrary accuracy ($\lambda\to 0$) and is deterministic? This would mean that quantum mechanics is a "singular point" in the set of possible "wave–particle" theories. Or, do peculiar quantum properties have to be attributed to systems with nonlinear laws of evolution?

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Elementary properties of a new kind of path integral

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A new kind of path integral is introduced. In ordinary quantum mechanics, it gives the projectors on the eigenspaces of the Hamiltonian. For parametrized systems, it represents a direct path integral version of the Dirac canonical quantization method by giving the projector on the physical space. Its properties on the most simple examples are studied. Applying it to quantum cosmology, the Hartle–Hawking wave function of the universe is recalculated.

I. INTRODUCTION

In recent years, we have witnessed a renaissance of the minisuperspace quantum cosmology. On one hand, this finite-dimensional model of quantum gravity is not charged with divergences, and one can study some principal problems like the time problem, the Hilbert space problem, the positivity problem, etc. (see, e.g., Ref. 1). On the other hand, if the model can be considered as some sort of approximation to the full theory, then one also obtains observable predictions like the inflationlike start of the universe,[2] the evolution of the observable structures,[3] etc.

Central for this development is the path integral method. In the present paper, we are going to define and investigate a path integral, which seems to be often used in quantum cosmology (e.g., Ref. 4) under the assumption that it gives the transition amplitude, but which, in fact, has a quite different meaning.

In Sec. II, we introduce this kind of path integral into ordinary quantum mechanics and study its properties with the help of two well-known simple models: a free nonrelativistic particle in one-dimensional space and a one-dimensional barrier penetration. We will see quite explicitly that the value of the path integral is independent of the regime, Lorentzian or Euclidean, that one is using to calculate it, and even that it, loosely speaking, chooses for itself the most suitable regime for the calculation.

In Sec. III, we show that our kind of path integral represents, in a quite straightforward way, the Dirac canonical quantization method for parametrized systems.[5] Thus, it is different from, and, in general, not equivalent to, the kind of path integrals that are rooted in the reduction canonical quantization method[6] (such path integrals are described, e.g., in Ref. 7). We shall also see how our path integral differs from that introduced by Teitelboim.[8] We study two well-known simple examples of parametrized systems: the free relativistic particle and the Robertson–Walker cosmological model with positive cosmological constant.

II. ORDINARY QUANTUM MECHANICS

A. General theory

Consider a time-independent Hamiltonian $\hat{H}$ acting on a space of functions of n variables. We shall generally use the rigged Hilbert space, consisting of the triple $\{H_0,H,H_1\}$ (see Ref. 9), where H_0 is the space $\mathcal{S}_n$ of rapidly decreasing functions on $\mathbf{R}^n$, H_1 is the space $\mathcal{S}'_n$ of tempered distributions, and H is the Hilbert space $L^2(\mathbf{R}^n)$ with the scalar product

$$(\psi,\varphi) = \int d^n q\, \psi^*(q^1,...,q^n)\varphi(q^1,...,q^n).$$

Let $\hat{H}$ be self-adjoint in H and let its spectrum $\sigma(\hat{H})$ contain a continuous part so that its eigenfunctions lie in H_1.

The motivation for using the rigged Hilbert spaces is that our main goal and object of study are the eigenspaces of $\hat{H}$ at some points of the continuous part of $\sigma(\hat{H})$, as it is, for example, the physical space of the Dirac canonical quantization method (see the cosmological section).

The space H_0 can be considered as a linear subspace of H, and H as a linear subspace of H_1. More precisely, there are linear maps i_0: $H_0 \to H$ and i_1: $H \to H_1$ defined by

$$i_0\varphi \equiv \text{class of functions equal to } \varphi \text{ almost everywhere}$$

and

$$\langle i_1\psi,\varphi \rangle = (\psi^*,i_0\varphi), \quad \forall\varphi\in H_0.$$

Here, $\langle \psi,\varphi \rangle$ denotes the value of the linear functional $\psi\in H_1$ at the point $\varphi\in H_0$.

An important property is that i_0H_0 is dense in H and that $\hat{H}H_0 \subset H_0$.

The eigenfunctions $\psi_{Ep}\in H_1$ of $\hat{H}$ are defined by

$$\langle \psi_{Ep},\hat{H}\varphi \rangle = E\langle \psi_{Ep},\varphi \rangle, \quad \forall\varphi\in H_0,$$

$E\in\sigma(H)$. Here p represents all other parameters that can label the eigenfunctions of $\hat{H}$ in the case of degeneration. The set $\{\psi_{Ep}\}$ is complete in the sense that every element of H_0 can be expanded as

$$(i_1\circ i_0)\varphi = \int_{\mathbf{R}^1} d\mu(E) \int_{B(E)} d\mu_E(p)\, c(E,p)\psi_{Ep}$$

with the property

$$(\varphi^*,\chi) = \int_{\mathbf{R}^1} d\mu(E) \int_{B(E)} d\mu_E(p)\, c(E,p)\langle \psi_{Ep},\chi \rangle,$$
$$\forall\chi\in H_0.$$

Here, $\mu(E)$ and $\mu_E(p)$ are suitable Stieltjes measures for summation over the spectrum of $\hat{H}$ and over the E-eigenspace basis labeled by p.

The set $\{\psi_{Ep}\}$ is also orthonormal in the sense that the coefficients $c(E,p)$ in the above expansion satisfy

$$c(E,p) = \langle \psi^*_{Ep},\varphi \rangle.$$

Let ψ_t be a one-parameter family of linear functionals

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from H_1 depending differentiably on t. We shall say that ψ_t satisfies the Schrödinger equation, if

$$i\frac{d}{dt}\langle\psi_t,\varphi\rangle = \langle\psi_t, i_0^{-1}\circ\hat{H}\circ i_0\varphi\rangle, \quad \forall\varphi\in H_0.$$

We have, then, the following property: If $(i_1\circ i_0)\,\varphi_t$ satisfies the Schrödinger equation in the above sense, then

$$i\frac{\partial}{\partial t}(i_0\varphi_t) = \hat{H}(i_0\varphi_t). \tag{1}$$

Let $K_t(q,q')$ be the kernel of the time development operator $e^{-it\hat{H}}$ in H; then, for any $\varphi\in H_0$, we define

$$\varphi_t(q) = \int d^n q'\, K_t(q,q')\varphi(q'),$$

so that φ_t satisfies the Schrödinger equation (1). We can construct K_t by means of the eigenfunction expansion:

$$(i_1\circ i_0)\varphi_t = \int_{\mathbf{R}^1} d\mu(E)\int_{B(E)} d\mu_E(p)\langle\psi^*_{Ep},\varphi\rangle\psi_{Ep}e^{-itE}.$$

Hence,

$$K_t(q,q') = \int_{\mathbf{R}^1} d\mu(E)e^{-itE}K_E(q,q'),$$

where we have defined

$$K_E(q,q') = \int_{B(E)} d\mu_E(p)\psi_{Ep}(q)\psi^*_{Ep}(q').$$

Roughly speaking, K_E is the projection operator on the eigenspace of $\hat{H}$ corresponding to the point $E\in\sigma(\hat{H})$. More precisely, for each $E\in\sigma(\hat{H})$, there is an operator $K_E: H_0\to H_1$ such that $K_E\,H_0$ is dense in the E-eigenspace of $\hat{H}$.

The inverse relation between K_E and K_t reads

$$K_E(q,q') = \frac{1}{2\pi}\left(\frac{d\mu(E)}{dE}\right)^{-1}\int_{\mathbf{R}^1} dt\, e^{iEt}K_t(q,q').$$

We express K_t as a path integral,

$$K_t(q,q') = \int d\mu[q(\tau)]e^{iI[q(\tau);t]}, \tag{2}$$

where $I[q(\tau);t]$ is the value of the action at the path $q=q(\tau)$, $\tau\in[0,t]$, $q(0)=q'$, $q(t)=q$. Then, we can write

$$K_E(q,q') = \left(\frac{d\mu(E)}{dE}\right)^{-1}\int_{\mathbf{R}^1}\frac{dt}{2\pi}\int d\mu[q(\tau)]e^{iS[q(\tau),t;E]}, \tag{3}$$

where

$$S[q(\tau),t;E] = I[q(\tau);t] + Et \tag{4}$$

is a "Legendre transform" of the action I. We must have, again, the boundary conditions

$$q(0)=q', \quad q(t)=q. \tag{5}$$

One can consider the right-hand side (rhs) of (3) as a new sort of path integral: it is the integral over *all* paths from q' to q without any restriction, whereas the rhs of (2) is an integral over all paths from q' to q with a fixed total time t. Equation (3) gives the interpretation of such an integral: it is the projector on the E-eigenspace of H.

The integral over t in (3) has to be defined more accurately: K_t is singular at $t=0$ and the contour of integration must go round the singularity through the lower complex t plane.

As the contour for the t integration is given, it becomes unimportant in which regime we calculate K_E. We can take the formula (3) as it stands and call this "Lorentz-regime calculation." Or, we can make the substitution $t=-it_E$ for t, integrate along the correspondingly rotated t_E contour, and call this "Euclidean-regime calculation." The expression that will appear in the exponent of the Euclidean path integral is given by

$$-S_E[q(\tau_E),t_E;E] = -I_E[q(\tau_E);t_E] + Et_E,$$

where I_E is the usual Euclidean action.

Hence, going over from one regime to another means nothing but a transformation of the time integration variables in the path integral (3) and the result remains unchanged by this. Let us stress this point once more by saying that it is not sensible (and even not possible) to continue analytically the obtained "propagator" from the Euclidean to the Lorentzian time (because it does not depend on time at all). We illustrate these properties by two simple examples.

B. Free particle in one-dimensional space

In this case, the formula (3) reduces to

$$K_E(x,x') = \frac{\sqrt{E}}{\pi}\int_C dt\frac{1}{\sqrt{4\pi it}}e^{i[(x-x')^2/4t+Et]}. \tag{6}$$

We have integrated over all $q(\tau)$, substituting

$$K_t(x,x') = (1/\sqrt{4\pi it})e^{i(x-x')^2/4t}$$

for $K_t(x,x')$ and

$$\frac{d\mu(E)}{dE} = \frac{1}{2\sqrt{E}}$$

for the measure. The mass of the particle is set equal to $\frac{1}{2}$.

Let us calculate the integral in (6) by the method of the steepest descent.[10] The corresponding formula reads

$$K_E(x,x') \cong \sum_{A=1}^{K}\frac{\sqrt{E}}{\pi}\frac{1}{\sqrt{4\pi it_A}}\sqrt{\frac{2\pi}{|\ddot{Q}_A|}}\,e^{iQ_A+i\alpha_A}, \tag{7}$$

where the index A numerates the saddle points, t_A is the value of t at the saddle point A, Q_A the value of the exponent

$$Q = (x-x')^2/4t + Et,$$

at t_A, $\ddot{Q}_A = (\partial^2 Q/\partial t^2)|_{t=t_A}$, and $\alpha_A = (\pi/4)\mathrm{sgn}(\ddot{Q}_A)$ (see Ref. 10).

We easily find that there are two saddle points $t_\pm$,

$$t_\pm = \pm|x-x'|/2\sqrt{E},$$

so that

$$Q_\pm = \pm\sqrt{E}\,|x-x'|,$$
$$\ddot{Q}_\pm = \pm 4E^{3/2}/|x-x'|,$$

and

$$\alpha_\pm = \pm\pi/4.$$

Setting this into (7), we obtain

$$K_E(x,x') \cong (1/2\pi)(e^{-i\sqrt{E}|x-x'|} + e^{i\sqrt{E}|x-x'|}),$$

or

$$K_E(x,x') \cong (1/\pi)\cos\sqrt{E}\,(x-x').$$

(This is exact!)

The saddle points lie at the real axis of the Lorentz time (or at the imaginary axis of the Euclidean time) and represent, therefore, Lorentzian classical solutions, the physical trajectories that begin at x', end at x, and have energy E:

$$q_{\pm}(\tau) = x' \pm \operatorname{sgn}(x-x')2\sqrt{E}\,\tau,$$
$$t = \pm |x-x'|/2\sqrt{E}.$$

C. Barrier penetration

Let $V(q)$ be a potential hill, $V(q)>0$ for all $q\in(-\infty,\infty)$, E a number such that $E<\operatorname{Max}_q V(q)$, and x',x chosen such that $x'<x$, $V(x)=V(x')=E$, and $V(q)>E$ for $q\in(x',x)$.

Let us calculate in the Euclidean regime. The Euclidean action reads

$$S_E[q(\tau),t;E] = \int_0^t d\tau \left[\frac{M}{2}\dot{q}^2 + V(q) - E\right],$$

where

$$q(0)=x', \quad q(t)=x.$$

The saddle points are the extremal paths of S_E:

$$\text{(a)} \quad \frac{\delta S_E}{\delta q(\tau)} = -M\ddot{q}(\tau) + V'(q(\tau)) = 0.$$

Multiplying by $\dot{q}(\tau)$, we obtain

$$-\tfrac{1}{2}M\dot{q}^2(\tau) + V(q(\tau)) = \text{const}, \quad \forall\tau, \tag{8}$$

$$\text{(b)} \quad \frac{\partial S_E}{\partial t} = \frac{M}{2}\dot{q}^2(t) + V(q(t)) - E + \int_0^t d\tau \frac{\delta S_E}{\delta q(\tau)}\frac{\partial q}{\partial t}(\tau) + \int_0^t d\tau \frac{\partial}{\partial\tau}\left[M\dot{q}(\tau)\frac{\partial q}{\partial t}(\tau)\right].$$

Setting this equal to zero and using the first equation, we have

$$\frac{M}{2}\dot{q}^2(t) + V(q(t)) - E + M\dot{q}(t)\frac{\partial q}{\partial t}(t) - M\dot{q}(0)\frac{\partial q}{\partial t}(0) = 0. \tag{9}$$

We need a relation between $\dot{q}$ and $\partial q/\partial t$. The extremal path $q(\tau)$ is also a function of t:

$$q = q(t,\tau)$$

with

$$q(t,0)=x', \quad q(t,t)=x',$$

for all t. Derivation of these equations with respect to t yields

$$\frac{\partial q}{\partial t}(t,0) = 0, \qquad \frac{\partial q}{\partial t}(t,t) + \frac{\partial q}{\partial\tau}(t,t) = 0, \tag{10}$$

that is,

$$\frac{\partial q}{\partial t}(t) = -\dot{q}(t). \tag{11}$$

Setting (10) and (11) into (9), and comparing with (8), we obtain

$$-\tfrac{1}{2}M\dot{q}^2(\tau) + V(q(\tau)) = E, \quad \forall\tau. \tag{12}$$

This is a classical Euclidean equation for a path $q(\tau)$ with a constant "Euclidean energy" E. The total time t along such a path, if it begins at x' and ends at x, is given by

$$t_{\pm} = \pm\int_{x'}^{x} dq \sqrt{\frac{M}{2[V(q)-E]}}. \tag{13}$$

The saddle is, therefore, at the real axis of the Euclidean time. As we must go round the singularity at 0 through the right half-plane, we can deform the contour only to go through t_+. The value of the exponent there is

$$S_E[q_+(\tau),t_+;E] = \int_0^{t_+} d\tau\left[\frac{1}{2}M\dot{q}_+^2(\tau) + V(q_+(\tau)) - E\right].$$

We can substitute for $\frac{1}{2}M\dot{q}_+^2$ from (8) and obtain

$$S_E[q_+(\tau),t_+;E] = 2\int_0^{t_+} d\tau[V(q_+(\tau)) - E].$$

Now, we change the integration variables from τ to q_+ using

$$\frac{dq_+}{d\tau} = +\sqrt{\frac{2[V(q_+)-E]}{M}}.$$

The result is

$$S_E(\text{extreme}) = \int_{x'}^{x} dq\sqrt{2M[V(q)-E]}.$$

Hence,

$$K_E(x,x') \sim \exp\left(-\int_{x'}^{x} dq\sqrt{2M[V(q)-E]}\right),$$

which is the desired formula.

III. PARAMETRIZED SYSTEMS

A. General theory

Consider the action of the form

$$I[q(\tau),\alpha(\tau);t] = \int_0^t d\tau\left(\frac{1}{2\alpha}g_{AB}\dot{q}^A\dot{q}^B - \alpha V\right), \tag{14}$$

where $\alpha(\tau)$ and $q^A(\tau)$, $A=1,\ldots,N$, are the dynamical variables, $g_{AB}(q^1,\ldots,q^N)$ is some metric, which is supposed to be nondegenerate, $g=\operatorname{Det}(g_{AB})\neq 0$, and $V(q^1,\ldots,q^N)$ is a potential. The space of variables $q^1,\ldots,q^N$ is usually called "superspace" or "minisuperspace."

For example, setting $q^A = x^\mu$, $g_{AB}=\eta_{\mu\nu}$, $\mu=0,1,2,3$, and $V=-\frac{1}{2}m^2$, we have an action of a free relativistic particle of mass m ($\eta_{\mu\nu}$ is the metric of Minkowski space-time).

If we choose $q^1=R$, $q^2=\phi$,

$$g_{11} = -3R/4\pi G, \quad g_{12}=0, \quad g_{22}=R^3,$$
$$V = (3k/4\pi G)R - m^2R^3\phi^2 - (\Lambda/3)R^3,$$

we have the Robertson–Walker cosmological model with the space-time line element

$$ds^2 = \alpha^2(t)dt^2 - R^2(t)\left(\frac{dr^2}{1-kr^2} + r^2\,d\Omega^2\right),$$

coupled minimally to a (spatially constant) Klein–Gordon scalar field $\phi(t)$. Here, G is the Newton constant, $k = \pm 1,0$ gives the sign of the curvature of space, m is the mass of ϕ, and Λ is the cosmological constant.

The action (14) is typical for *relativistic* systems. Thus, the parametrized action of a nonrelativistic particle in a potential will not be of this form.

The generalized momenta are defined by

$$p_A = \frac{\partial L}{\partial \dot{q}^A} = \frac{1}{\alpha} g_{AB}\, \dot{q}^B,$$

$$p_\alpha = \frac{\partial L}{\partial \dot{\alpha}} = 0.$$

The constraint $\mathscr{H}_0$ is obtained as follows:

$$\mathscr{H}_0 = -\frac{\delta I}{\delta \alpha(\tau)} = \frac{1}{2\alpha^2} g_{AB}\dot{q}^A\dot{q}^B + V$$
$$= \tfrac{1}{2} g^{AB} p_A\, p_B + V,$$

and the Hamiltonian H is defined by

$$H = \dot{q}^A p_A - L = \alpha \mathscr{H}_0.$$

There are essentially two different methods of quantizing this system canonically: the reduction method and the Dirac method (see, e.g., Ref. 6).

The Dirac method consists of taking $L^2(\mathbf{R}^N)$ as an auxiliary Hilbert space and associating the operators $\hat{q}^A$ and $\hat{p}_A$ with all $2N$ variables q^A and p_A as if they were independent; q^A and p_A are defined on $\mathscr{S}_N$, the space of rapidly decreasing functions as follows: if $\psi(q) \in \mathscr{S}_N$, then

$$\hat{q}^A\psi(q) = q^A\psi(q),$$

$$\hat{p}_A\psi(q) = -i\frac{\partial}{\partial q^A}\psi(q).$$

One can extend these operators to self-adjoint ones on $L^2(\mathbf{R}^n)$. Next, one rewrites the constraint $\mathscr{H}_0$ by substituting the operators $\hat{q}^A$ and $\hat{p}_A$ for q^A and p_A into it, choosing the factor ordering such that $\hat{\mathscr{H}}_0$ is (a) symmetric in $L^2(\mathbf{R}^n)$ and (b) independent of the choice of coordinates q^A. This leads to

$$\hat{\mathscr{H}}_0 = -\tfrac{1}{2}(1/\sqrt{|g|})\partial_A\sqrt{|g|}\, g^{AB}\partial_B + \xi\mathscr{R} + \eta + V,$$

where ξ and η are arbitrary real constants and $\mathscr{R}$ is the curvature scalar of g_{AB}.

Then, the constraint is implemented by the following condition on states:

$$\hat{\mathscr{H}}_0\psi = 0. \tag{15}$$

This is the celebrated Wheeler–DeWitt equation. The solutions of (15) are called "physical states" and the set of all physical states is called "physical (Hilbert) space" H_p.

A difficulty arises at this stage. For most potentials V, zero is a point of the continuous part of the spectrum $\sigma(\hat{\mathscr{H}}_0)$ of the self-adjoint extension of $\hat{\mathscr{H}}_0$. Thus, the solutions of (15) do not lie in $L^2(\mathbf{R}^N)$. If one assumes that $H_p \subset L^2(\mathbf{R}^N)$ and that the scalar product on H_p is identical with that of $L^2(\mathbf{R}^N)$, one obtains strange paradoxes.[11] Hence, we must take the rigged Hilbert space, $\{H_0, H, H_1\}$, where

$$H_0 = \mathscr{S}_N, \quad H = L^2(\mathbf{R}^N), \quad H_1 = \mathscr{S}^1_N,$$

consider H_p as a subspace of H_1, and introduce a scalar product on H_p, which is independent of the auxiliary scalar product on H (using, say, the conserved current associated with the Wheeler–DeWitt equation, see, e.g., Ref. 1).

Our main point is based on the observation that the constraint $\mathscr{H}_0$ and the Hamiltonian H are proportional to each other, if α is chosen to be a fixed (but arbitrary) function of t. We can, therefore, directly represent the Dirac quantization method by path integrals as follows. Let us introduce an auxiliary dynamics on H by the Schrödinger equation

$$i\frac{\partial\psi}{\partial\tau} = \alpha(\tau)\hat{\mathscr{H}}_0\psi. \tag{16}$$

This is the Schrödinger equation that corresponds to the action (14), if the variable α in (14) is replaced by a fixed function $\alpha(\tau)$ of time. Equation (16) can be written

$$i\frac{\partial\psi}{\partial t} = \hat{\mathscr{H}}_0\psi, \tag{17}$$

where

$$t = \int_0^\tau dx\, \alpha(x). \tag{18}$$

The Schrödinger equation (17) has a time-independent Hamiltonian $\hat{\mathscr{H}}_0$. The kernel $K_p(q,q')$ of the projection operator on the 0-eigenspace of $\hat{\mathscr{H}}_0$ is, therefore, given by the path integral:

$$K_p(q,q') = \frac{1}{2\pi}\left(\frac{d\mu(E)}{dE}\right)^{-1}_{E=0}\int_C \alpha(t)dt \int d\mu[q(\tau)]$$
$$\times e^{iI[q(\tau),\alpha(\tau);t]}. \tag{19}$$

Here, for $\alpha(\tau)$ or $\alpha(t)$, a fixed function must be inserted. This means that we allow only this particular class of gauge conditions. The result will be independent of the choice.

There are two interesting problems, which are not difficult to solve, but which will not be dealt with in the present paper.

(1) Extend the path integral formulation of the Dirac method, as given by (19), to a more general class of gauge conditions. That is, for example, a gauge condition of the form

$$\chi(q^A, p_A) = 0.$$

(2) Extend the path integral formulation (19) of the Dirac method to parametrized systems with more than one parameter. Thus, there will be more constraints, the Hamiltonian will be a linear combination of them (like in general relativity), and the 0-eigenspaces of it will not coincide with the physical space any more.

We illustrate the formula (19) by two simple examples.

B. Free relativistic particle

In this example, we will see that, by our method, we will obtain the projection operator on the *whole* of the "physical space," even if it is highly degenerated. Also, we obtain the projection operator on the space of *all* solutions of the Klein–Gordon equation and not just on the *positive* frequency solution or other interesting subspaces, as it would be the case with other sorts of propagators.

We will work in the momentum representation and choose $\alpha = 1$. Thus, the auxiliary dynamics is

$$i\frac{\partial\psi}{\partial t} = \frac{1}{2}(\eta^{\mu\nu}p_\mu p_\nu - m^2)\psi,$$

where $\psi = \psi(t,\mathbf{p})$, $\mathbf{p}\equiv(p_0,p_1,p_2,p_3)$. This can be immediately integrated to give

$$K_t(\mathbf{p},\mathbf{p}') = e^{-(i/2)(p^2-m^2)\tau}\delta^4(\mathbf{p}-\mathbf{p}'),$$

where $K_t(\mathbf{p},\mathbf{p}')$ is the kernel of $e^{-it\hat{H}_0}$ and $p^2 = \eta^{\mu\nu}p_\mu p_\nu$.

Then, according to our recipe,

$$\left(\frac{d\mu(E)}{dE}\right)_{E=0} K_p(\mathbf{p},\mathbf{p}') = \lim_{\epsilon\to 0+}\frac{1}{2\pi}\int_{-\infty}^{\infty} dt\exp\left[-\frac{i}{2}(p^2-m^2)t - \frac{\epsilon}{2}t^2\right]\delta^4(\mathbf{p}-\mathbf{p}')$$

$$= \lim_{\epsilon\to 0+}\frac{1}{\sqrt{2\pi\epsilon}}\exp\left[-\frac{(p^2-m^2)^2}{8\epsilon}\right]\delta(\mathbf{p}-\mathbf{p}') = 2\delta(p^2-m^2)\cdot\delta^4(\mathbf{p}-\mathbf{p}').$$

This is the desired result.

We can see from it, moreover, what is the difference between our path integral and that introduced by Teitelboim: the latter will give the causal propagator for the Klein–Gordon field.[8]

It is not clear whether such a "causal propagator" is desirable or sensible in general relativity. As Misner very clearly explained,[12] there is no necessity for classical trajectories to lie inside the "light cones" of the superspace metric g_{AB}, and so there is no physically relevant time orientation of the superspace. The Wheeler–DeWitt equation has twice as many solutions as a Schrödinger equation would have, because the former is real, whereas the latter is complex. All of these solutions are physical; the time orientation of a given state is determined by the corresponding value of the Wheeler–DeWitt conserved current.

C. The wave function of the universe

In this section, we are going to illustrate two points.

(1) The path integral (19) does *not* yield, in general, a theory equivalent to that obtained from the *usual* path integral for parametrized systems. By "usual," we mean the construction described in Ref. 7, which starts by the path integral expression for the propagator of the *reduced* theory. It is well known that the reduction method and the Dirac method of canonical quantization can give different results. One (a little artificial) example of it has been described in Ref. 13. Here, we shall give another, even simpler, example, which is, moreover, directly relevant to quantum cosmology.

(2) On recalculating the wave function of the universe by our method, we show that our path integral coincides, in fact, with that which is calculated in Ref. 4. This may seem surprising at first sight, because Hartle and Hawking arrived at their integral by "generalizing" the path integral formula for the transition amplitude to the parametrized system. The end result of this generalization is as follows: one fixes two three-geometries, h'_{ij} and h_{ij}, say, and then integrates over all four-geometries that contain h'_{ij} and h_{ij} as their boundary. However, such a path integral does naturally include the sum over all proper time distances between h'_{ij} and h_{ij}. It will not, therefore, give the transition amplitude between h'_{ij}, and h_{ij} but rather the projection operator on the physical space.

In our calculation, we will consider the system with the action (14), in which we set $\phi\equiv 0$, $k = 1$, and $\Lambda > 0$. Instead of Λ, we shall use a length parameter a defined by

$$a = \sqrt{3/\Lambda}.$$

As it is well known, the corresponding classical theory has no dynamics of its own, all degrees of freedom being dependent, and all "dynamical" information being contained in the constraint:

$$\mathscr{H}_0 = -(R/\alpha^2)\dot{R}^2 - kR + a^{-2}R^3 = 0.$$

The only classical solution to this constraint is the de Sitter space-time of radius a. Still, the Dirac method of quantization can be formally applied, giving a nontrivial Hilbert space $H = L^2(\mathbb{R}^1)$, and a nontrivial Wheeler–DeWitt equation. This will be an *ordinary* differential equation and the corresponding physical space will have finite dimension. We shall see, however, a typical way that the Dirac method allows tunneling into regions forbidden by the classical constraint.

Let us set $\alpha = 1$ and rewrite the formula (19) in a way corresponding to our system:

$$K_p(R,R') \sim \int_C dt\int d\mu[\rho(\tau)] \times\exp\left(\frac{3i}{4\pi G}\int_0^t d\tau(-\rho\dot{\rho}^2 + \rho - a^{-2}\rho^3)\right),$$

where $\rho(0) = R'$, $\rho(t) = R$. Following Hartle and Hawking,[4] we choose $R' = 0$, obtaining a function $\psi(R) = K_p(R,0)$, which will be interpreted as the wave function of the universe.

Let us calculate $\psi(R)$ by the method of steepest descent. The saddle points are the extremal paths of the action. Variation with respect to $\rho(\tau)$ and t leads to the differential equation for the extremal paths:

$$\rho\dot{\rho}^2 + \rho - a^{-2}\rho^3 = 0.$$

This is nothing but the constraint; t must satisfy the conditions

$$\rho(0) = 0, \quad \rho(t) = R,$$

where R is fixed.

Distinguish two cases: (A) $R \leqslant a$, and (B) $R > a$.

(A) We have four solutions of the form

$$\rho = a\sin\frac{\sigma}{a}, \quad \tau = i\epsilon\sigma, \quad t = i\epsilon\left(\frac{a\pi}{2} + \eta a\arccos\frac{R}{a}\right),$$

$$0 \leqslant \sigma \leqslant a\pi/2 + \eta a\arccos(R/a),$$

where ϵ and η are given, in the four different cases, by

(A1) $\epsilon = +1, \quad \eta = +1,$

(A2) $\epsilon = +1, \quad \eta = -1,$

(A3) $\epsilon = -1, \quad \eta = +1,$

(A4) $\epsilon = -1, \quad \eta = -1,$

and we define the arccos x to satisfy $0 < \arccos x < \pi/2$.

The corresponding metrics are metrics of the Euclidean four-sphere with radius a and with an S^3 boundary of radius R:

$$ds^2 = -d\sigma^2 - a^2 \sin^2(\sigma/a)(dr^2/(1-r^2) + r^2\, d\Omega^2).$$

(B) We have again four solutions, this time of the form

$$0 < \sigma < a\pi/2: \qquad \rho = a \sin\frac{\sigma}{a},$$

$$\tau = i\epsilon\sigma,$$

$$\frac{a\pi}{2} < \sigma < \frac{a\pi}{2} + a\,\operatorname{arccosh}\frac{R}{a}: \qquad \rho = a\cosh\left(\frac{\sigma}{a} - \frac{\pi}{2}\right),$$

$$\tau = i\frac{\epsilon a\pi}{2} + \eta\left(\sigma - \frac{a\pi}{2}\right),$$

$$t = i\frac{\epsilon a\pi}{2} + \eta a\,\operatorname{arccosh}\frac{R}{a},$$

where ϵ and η are given by

(B1) $\epsilon = +1, \quad \eta = +1,$

(B2) $\epsilon = +1, \quad \eta = -1,$

(B3) $\epsilon = -1, \quad \eta = +1,$

(B4) $\epsilon = -1, \quad \eta = -1,$

and $\operatorname{arccosh} x = \log(x + \sqrt{x^2 - 1})$.

The metrics in all four cases are those of the well-known Vilenkin solutions.[14]

The extremal values of the action are given by

$$\text{(A)} \quad iI = -\epsilon\frac{a^2}{2\pi G} - \epsilon\eta\frac{a^2}{2\pi G}\left(\sqrt{1 - \frac{R^2}{a^2}}\right)^3,$$

$$\text{(B)} \quad iI = -\epsilon\frac{a^2}{2\pi G} - i\eta\frac{a^2}{2\pi G}\left(\operatorname{arccosh}\frac{R}{a}\right)^3.$$

We will approximate the function ψ by the sum of the exponential expressions over the saddle points.

The kinetic term $\rho\dot{\rho}^2$ in the action has an unusual sign. Thus, we have to lay the integration contour in the t plane above the real axis near $t = 0$, and so the contour can be deformed to go only through the saddle points that are above the real axis. These are the cases (A1), (A2), (B1), and (B2). Hence, the wave function has the form

$$\psi(R) \sim e^{iI(\text{A1})} + e^{iI(\text{A2})}$$

$$= 2e^{-a^2/2\pi G}\cosh\left[\frac{a^2}{2\pi G}\left(\sqrt{1 - \frac{R^2}{a^2}}\right)^3\right],$$

for $R < a$,

$$\psi(R) \sim e^{iI(\text{B1})} + e^{iI(\text{B2})}$$

$$= 2e^{-a^2/2\pi G}\cos\left[\frac{a^2}{2\pi G}\left(\operatorname{arccosh}\frac{R}{a}\right)^3\right],$$

for $R > a$. (20)

We observe that ψ equals ~ 1 at $R = 0$ and has a local maximum there, then falls off exponentially, tunneling through the classically forbidden region, till it reaches the value $2e^{-a^2/2\pi G}$ at $R = a$, the smallest classically allowed radius; $d\psi/dR\,(a) = 0$. Then, ψ is given by a linear combination of two semiclassical solutions corresponding to de Sitter space-time with two opposite time orientations. The wave function (20) can be interpreted as describing a spontaneous coming of the universe into being, the probability being $\sim e^{-a^2/2\pi G}$. Notice, however, that, at least for the present model, no explanation of the origin of the universe is really required, because the classical solution, the de Sitter space-time, is eternal in both time directions.

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On the summation of the Birkhoff–Gustavson normal form of an anharmonic oscillator

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The classical Birkhoff–Gustavson normal form (BGNF) has played an important role in finding approximate constants of motion, and semiclassical energies. In this paper, this role is examined in detail for the well-known anharmonic oscillator $H = 1/2(p^2 + x^2 + gx^4)$. It is shown that, with appropriate restrictions, this is the only perturbation series that preserves the period of this system. This series has a nonzero radius of convergence in contrast to the zero radius of convergence of its quantum analog, the Rayleigh–Schrödinger perturbation series. In addition, the BGNF is generated to high order, and a technique is given based on Padé approximants for summing this series. The summation of this series makes possible an accurate comparison of torus quantization energies with the known quantum energies over the entire range of quantum numbers. This example also demonstrates that divergence of the BGNF series of a Hamiltonian is not sufficient to refute its global integrability.

I. INTRODUCTION

The classical Birkhoff–Gustavson normal form[1,2] (BGNF) has received considerable attention[2–5] in finding approximate constants of motion and semiclassical energies of nonlinear Hamiltonian systems. In our recent work[6] on the quantum normal form, we have shown that there exists an algebraic connection between the BGNF and the Rayleigh–Schrödinger perturbation (RSP) theory. The role played by the BGNF in classical mechanics is equivalent to that of the RSP in quantum mechanics. In addition, quantization of the BGNF by techniques such as torus and Weyl quantizations[3,6] are straightforward. Therefore, the BGNF, which is derivable by the technique of Lie transforms,[7–10] is of special importance among all possible perturbation methods of classical mechanics and it is worthwhile to look at the BGNF in detail for some model system.

Until now, applications of the BGNF have been restricted to relatively low order approximations.[2–6] In their work on vague tori, Shirts and Reinhardt[4] generated, through the introduction of a simplification, the first ten terms in the BGNF series for the two-dimensional Hénon–Heiles and Toda systems and summed the "direct" ten-term series by employing the Padé approximant technique. (We are grateful to the referee for drawing our attention to this summation of a BGNF by the Padé approximant approach.) However, in their work on the summation, they found that additional terms would be "highly desirable." Also, in applying the BGNF approach, the convergence properties of the series in question have not been sufficiently emphasized. In practice, the BGNF series may diverge, as illustrated later on, even for simple integrable[11] systems.

The objectives of this work are (1) to generate and sum the BGNF series of a model anharmonic oscillator, (2) to present the solution in a form suitable for addressing an old and fundamental question of how to quantize a classical system in which the coordinates and momenta do not appear in a simple manner, (3) to provide additional evidence emphasizing the special importance of the classical BGNF perturbation method, and (4) to compare the anharmonic oscillator energies obtained by quantum calculations and by torus quantization of the BGNF.

Algebraic and exact computations have played a crucial role throughout all phases of this investigation. All computation, numerical or otherwise, reported in this paper has been carried out using the MAPLE[12] symbolic algebra system.

II. THE BGNF OF AN ANHARMONIC OSCILLATOR

The Hamiltonian of the anharmonic oscillator of our present work is obtained by substituting $b = 0$ in Eqs. (24)–(27) of our earlier work.[6] That is

$$H = H_0 + H_1 + H_2/2, \quad H_0 = \tfrac{1}{2}(p^2 + x^2), \quad H_1 = bx^3, \quad H_2 = gx^4, \quad b = 0, \quad g \geqslant 0. \tag{1}$$

This Hamiltonian has been extensively studied as a mathematical and physical model[13–47] in classical and quantum theories. The exact solution[14–16] of Newton's equation of motion for H is known in terms of Jacobi elliptic functions, and the period and action of this classical problem have been reported in terms of generalized hypergeometric functions.[13] Some approximate solutions[16,17] of Newton's equation are also available in the literature. However, none of the currently existing solutions are in a convenient form for studying the fundamental quantization problem. The BGNF approach not only provides the solution of the classical equation of motion but also yields the solution in a form that is suitable for applying known quantization procedures.

The work[19–47] on the solutions of the Schrödinger equation for the anharmonic oscillator is more extensive than on its classical counterpart. While detailed analysis[31,37,38,43,45,46] of the convergence of the RSP series for the problem is available in the literature, such is not the case for

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the BGNF, the classical analog of the RSP. In our present work we fill this gap.

In the BGNF approach, the Hamiltonian $H(x,p)$ is transformed[2] to the normal form $K(\xi,\eta)$ by a canonical transformation of the phase space variables (x,p) to the variables (ξ,η). The Hamiltonian $H(x,p)$ is assumed to have the form

$$H(x,p) = \sum_{n=0}^{M} \frac{H_n}{n!},$$

where the $H_n(x,p)$ are homogeneous polynomials of degree $n+2$ in x and p and $M \geqslant 0$. The normal form $K(\xi,\eta)$ is

$$K = \sum_{n=0}^{\infty} \frac{K_n}{n!}, \tag{2}$$

where the K_n are homogeneous polynomials of order $n+2$ in ξ, η and the Poisson brackets $\{K_0,K_m\} = 0$ for all m. The required canonical transformation is carried out using the method of Lie transforms for which the details are given in the earlier paper.[6] The first few terms of the series, Eq. (2), obtained using Lie transforms in this manner are

$$K_0 = H_0,$$
$$K_1 = H_1 + \{H_0,w_1\},$$
$$K_2 = H_2 + 2\{H_1,w_1\} + \{H_0,w_2\} + \{\{H_0,w_1\},w_1\},$$

where $\{A,B\}$ represents the Poisson bracket of A and B and the generating function $w(\xi,\eta)$ is given by

$$w(\xi,\eta) = \sum_{n=0}^{\infty} \frac{w_{n+1}(\xi,\eta)}{n!}.$$

Here the $w_{n+1}(\xi,\eta)$ are homogeneous polynomials of degree $n+3$ in ξ and η. The K_n and w_{n+1} are determined from the equations of the Lie transforms and the condition $\{K_0,K_m\} = 0$ for all m. We have set $b = 0$ (i.e., $H_1 = 0$) and $g \geqslant 0$.

The advantage of using the Lie transform is that a connection[6] between the BGNF and RSP follows when the Poisson brackets of the BGNF are replaced by the corresponding commutators. A partial result generated by this method for the series in Eq. (2) is $K = UK_0$, where

$$\begin{aligned} U = 1 &+ \frac{3y}{4} - \frac{17y^2}{16} + \frac{375y^3}{128} - \frac{10\,689y^4}{1024} + \frac{87\,549y^5}{2\,048} - \frac{3132\,399y^6}{16\,384} + \frac{238\,225\,977y^7}{262\,144} - \frac{18\,945\,961\,925y^8}{4\,194\,304} \\ &+ \frac{194\,904\,116\,847y^9}{8388\,608} - \frac{8\,240\,234\,242\,929y^{10}}{67\,108\,864} + \frac{11\,128\,512\,976\,035y^{11}}{16\,777\,216} - \frac{15\,671\,733\,036\,451\,359y^{12}}{4294\,967\,296} \\ &+ \frac{87\,535\,900\,033\,269\,525y^{13}}{4294\,967\,296} - \frac{7925\,536\,921\,177\,219\,335y^{14}}{68\,719\,476\,736} + \frac{1451\,374\,598\,407\,735\,283\,589y^{15}}{2199\,023\,255\,552} \\ &- \frac{268\,400\,255\,715\,098\,864\,816\,085y^{16}}{70\,368\,744\,177\,664} + \frac{3129\,005\,835\,033\,377\,759\,527\,767y^{17}}{140\,737\,488\,355\,328} \\ &- \frac{147\,029\,573\,283\,245\,261\,933\,818\,725y^{18}}{1\,125\,899\,906\,842\,624} + \frac{1739\,007\,165\,801\,666\,889\,770\,104\,925y^{19}}{2251\,799\,813\,685\,248} \\ &- \frac{331\,111\,612\,436\,057\,226\,338\,390\,665\,719y^{20}}{72\,057\,594\,037\,927\,936} + \frac{1981\,052\,002\,445\,082\,082\,574\,905\,382\,175y^{21}}{72\,057\,594\,037\,927\,936} \end{aligned} \tag{3}$$

and

$$y = gK_0, \quad K_0 = \tfrac{1}{2}(\xi^2 + \eta^2). \tag{4}$$

The BGNF series, Eq. (3), for the integrable anharmonic oscillator of Eq. (1) has a positive radius of convergence y_0, as compared to the zero radius of convergence[22,37,41,45] of its quantum analog the RSP series. The questions of determination of y_0 and summation of the series for K will be discussed below. The divergence for $y \geqslant y_0$ of the series in Eq. (3), even though the associated anharmonic oscillator is integrable, demonstrates that the divergence of the BGNF series of a Hamiltonian is not sufficient for ascertaining its global nonintegrability.

In terms of the BGNF, the dynamics of the anharmonic oscillator is essentially reduced to that of a harmonic oscillator. This can be seen by considering the action

$$I = K_0 \tag{5}$$

and Hamilton's canonical equations of motion

$$\frac{d\xi}{dt} = \omega\eta,$$
$$\frac{d\eta}{dt} = -\omega\xi, \tag{6}$$

where

$$\omega = \frac{dK}{dK_0} = \text{a constant for a given } K_0. \tag{7}$$

The above equations of motion are the same as those of a harmonic oscillator with the Hamiltonian

$$\kappa = (\omega/2)(\xi^2 + \eta^2). \tag{8}$$

The main difference between the equations of motion of the anharmonic oscillator, Eqs. (6), and those of the harmonic oscillator with Hamiltonian κ is that for the anharmonic oscillator the ω depends on the action I and hence on K, while for the harmonic oscillator the ω is independent of ξ and η. However, for every given I the ω is fixed and the time evolution of the coordinate and momentum of the anharmonic oscillator is that of a harmonic oscillator with the

corresponding ω. This simple relationship for the dynamics of the anharmonic oscillator combined with the summation of the BGNF series will be utilized in a following paper addressing the quantization question.

III. THE SUMMATION OF THE BGNF SERIES

As mentioned earlier, the normal form series, Eq. (3), diverges when $y \geqslant y_0$. We now discuss how to determine y_0 and find expressions for K that are valid for all $y \geqslant 0$. Summation techniques such as Padé[48] and Borel–Padé[49,50] suggest themselves since these techniques have been successfully applied by earlier workers[37,47] to the analogous RSP series of the anharmonic oscillator.

A. The Padé and Borel–Padé summation of the BGNF

Before applying these summation techniques, it is instructive to look at the asymptotic behavior of K as $y \to \infty$. From a first-order WKBJ calculation,[51] which is valid for large quantum numbers n, and considering the validity of the semiclassical torus quantization, $K_0 = n + \frac{1}{2}$, one finds the limiting values (see also Sec. III B)

$$\lim_{y\to\infty} U = CK_0^{1/3} \quad \text{and} \quad \lim_{y\to\infty} K = CK_0^{4/3}, \tag{9}$$

where

$$C = \alpha^{4/3} g^{1/3}, \quad \alpha = 3\Gamma(\tfrac{3}{4})^2/\pi^{1/2}2^{5/4}. \tag{10}$$

We also have the lower limits $U = 1$ and $K = K_0$ as $y \to 0$. A valid summation technique must yield these limiting values for U and K.

Because of the fractional powers of K_0 in Eqs. (9), the Padé sum of the "direct" series, Eq. (3), will fail to produce the correct asymptotic value of K. For example, the incorrect behavior of the $[m,m]$, $[m,m+1]$, and $[m+1,m]$ Padé approximants of this direct series is illustrated in Fig. 1. Thus, in what follows, we will not deal with the Padé approximants of the direct series.

The $\frac{1}{3}$ power of K_0 in U suggests that instead of working with the direct series, we should calculate the $[m+1,m]$ Padé approximants, $P[m+1,m]$, for $Z = U^3$. Then

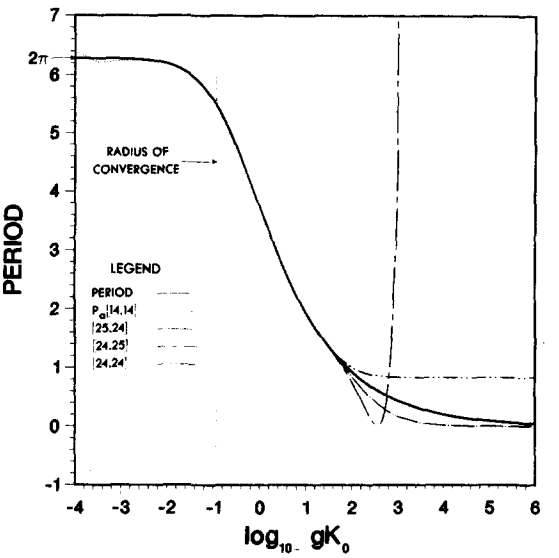

FIG. 1. Comparison of the exact period with those determined from various Padé approximants. The period for $P[14,13]$ coincides almost exactly with the exact period and is not visible. The period for $P_a[14,14]$ deviates from the exact period for low values of $y = gK_0$, while each of the [24,25], [25,24], and [24,24] Padé approximants of the direct series deviate significantly outside the radius of convergence $y \approx 0.116$.

$$Z \approx P[m+1,m] \tag{11}$$

and

$$K \approx K_0\{P[m+1,m]\}^{1/3}. \tag{12}$$

The terms of Z are inaccurate beyond the chosen order of U. For our purposes a choice of order 50 was more than adequate and we have used this to obtain $P[2,1]$, $P[3,2]$,...,$P[25,24]$. The coefficients for $P[14,13]$, given in Table I, yield $Z \approx P[14,13]$ and $K \approx K_0\{P[14,13]\}^{1/3}$.

If the sequence of Padé approximants converges, then any desired accuracy in K can be obtained by an appropriate choice for the value of m. Our numerical results suggest that

TABLE I. Coefficients of the [14,13] Padé approximant, $P[14,13] = \{\sum_{i=0}^{14} c_i y^i\}/\{\sum_{i=0}^{13} d_i y^i\}$ of the series Z associated with Eq. (3). The normal form K is given by setting $m = 13$ in Eq. (12).

i	c_i	d_i
0	1.000 000 000 000 0000000	1.000 000 000 000 0000000
1	44.831 784 212 934 880188	42.581 784 212 934 880188
2	898.880 683 944 016 77951	804.571 624 464 913 29908
3	10 639.165 060 022 835 342	8 888.321 893 796 182 7393
4	82 640.647 992 903 648 310	63 676.695 257 241 372 118
5	443 020.526 179 025 895 32	310 150.585 440 022 009 38
6	1 678 200.116 692 228 089 6	1 047 147.533 089 756 735 5
7	4 523 026.628 791 581 046 9	2 452 852.612 586 951 997 3
8	8 617 937.258 956 140 827 5	3 926 329.085 240 141 660 5
9	11 383 768.694 822 983 447	4 155 451.165 437 315 718 9
10	10 061 467.373 625 541 364	2 744 725.555 003 753 572 5
11	5 611 136.004 484 921 306 3	1 024 710.372 500 140 240 7
12	1 789 539.665 080 642 886 7	179 818.300 386 857 591 76
13	272 303.169 746 185 049 47	9 642.611 655 328 590 2038
14	12 965.942 908 295 871 194	

(1) the Padé sequence for Z converges, (2) there are no zeros or poles of the $P[m+1,m]$ on the positive real axis ($y>0$), (3) as $y\to\infty$, the $P[m+1,m]$ with increasing m yield results that approach the asymptotic values given by Eqs. (9), and (4) the Padé sequence yields better results for smaller y. We have also performed the Borel–Padé summation for K, which gives slightly better results than $P[m+1,m]$ for any given m. For example, the Borel–Padé sum obtained using Z with any given m will be comparable with the Padé sum obtained by $P[m+3,m+2]$. However, the gain in the Borel–Padé approach[47] is offset, for the present system, by the necessary extra numerical work and hence our Borel–Padé results will not be discussed further in this paper.

Although the sequence of Padé approximants converges as m increases and gives, at least in principle, *the sum of the BGNF series*, the rate of convergence of the sequence is rather slow when y becomes large. For example, at $y=\infty$, $P[14,13]$ and $P[25,24]$, respectively, give the values 1.076 84 and 1.072 53 for the constant α, Eq. (10), while the exact value for this constant to six figures is 1.068 63. We therefore present a second expression for the sum of K that converges faster as y becomes larger. This additional expression is based on a connection between the BGNF and generalized hypergeometric functions.

B. The BGNF and generalized hypergeometric functions

Recently, Codaccioni and Caboz[13] have worked out the period of the anharmonic oscillator in terms of the hypergeometric function $F(\frac{1}{4},\frac{3}{4},1;-8gE)$, where E is the total energy. If E is a function of K_0, it is a simple matter to relate K_0 to E by using this hypergeometric function. By Hamilton's canonical equations of motion, the period of the classical motion is

$$T=\frac{2\pi}{\Omega},\quad \Omega=\frac{dE}{dK_0}.$$

Using the results of Codaccioni and Caboz we obtain

$$\Omega=\frac{dE}{dK_0}=\frac{1}{F(\frac{1}{4},\frac{3}{4},1;-8Y)},\quad Y=gE,$$

which has the solution

$$K_0=EF(\tfrac{1}{4},\tfrac{3}{4},2;-8Y),$$

in agreement with the equation for the action given by Codaccioni and Caboz. The unique power series solution for E (in powers of K_0) of this functional equation turns out to be the BGNF series K. Thus, at least for the anharmonic oscillator under consideration, the BGNF series is the unique series for K in powers of K_0, which represents the period exactly. This provides strong additional evidence emphasizing the special role played by the BGNF perturbation method.

Setting $E=K$ in the above equations, we obtain

$$T=\frac{2\pi}{\omega},\quad \omega=\frac{dK}{dK_0}, \tag{13}$$

$$\frac{dK}{dK_0}=\frac{1}{F(\frac{1}{4},\frac{3}{4},1;-8Y)},\quad Y=gK, \tag{14}$$

and

$$K_0=KF(\tfrac{1}{4},\tfrac{3}{4},2;-8Y). \tag{15}$$

Since the hypergeometric function[52,53] $F(\frac{1}{4},\frac{3}{4},2;-8Y)$ converges for $Y<\frac{1}{8}$, we obtain the radius of convergence y_0 of the BGNF series by solving the equation

$$gK=\tfrac{1}{8}. \tag{16}$$

Using Eq. (12) for K and since $y=gK_0$, Eq. (16) gives

$$y\{P[14,13]\}^{1/3}=\tfrac{1}{8}. \tag{17}$$

The physically acceptable solution of Eq. (17) gives the radius of convergence $y_0=0.116\ 162\ 780\ 721\ 1097$. This is in contrast to the RSP series, the quantum analog of the BGNF series, which has a radius of convergence of zero.

To find a valid expression for K in the range $y_0<y\leqslant\infty$, the hypergeometric function of Eq. (15) is analytically continued[52,53] to obtain

$$y=\frac{Y^{3/4}}{\alpha}F\left(\frac{1}{4},-\frac{3}{4},\frac{1}{2};-\frac{1}{8}Y\right)-\frac{3\Gamma(\frac{3}{4})^4Y^{1/4}}{\pi^2\alpha 2^{3/2}}F\left(\frac{3}{4},-\frac{1}{4},\frac{3}{2};-\frac{1}{8}Y\right). \tag{18}$$

The reversion of the series in Eq. (18) is complicated by the fractional powers of Y. In order to overcome this difficulty, we expand the F's of Eq. (18) in series to order N, set $z=(\alpha y)^{-2/3}$ and $W=Y^{-1/2}$, and expand the expression $z=W[\Sigma_{i=0}^{N}a_iW^i]^{-2/3}$ to order N. This allows us to determine the Lagrange series[54,55] for W and hence for Y. Finally, the reversion gives K in terms of K_0 as

$$K=\sum_{i=0}^{\infty}c_iz^i,\quad z=(\alpha y)^{-2/3}. \tag{19}$$

A partial sum of this infinite series appears as

$$\begin{aligned}K=\frac{1}{gz^2}\Bigg\{&1-\frac{4c}{3}z+\left(\frac{2c^2}{3}-\frac{1}{16}\right)z^2-\frac{8c^3}{81}z^3-\left(\frac{5c^4}{243}-\frac{1}{3\,072}\right)z^4+\frac{c}{1\,920}z^5+\left(\frac{14c^6}{6561}+\frac{7c^2}{13\,824}\right)z^6\\&+\left(\frac{16c^7}{19\,683}+\frac{7c^3}{19\,440}\right)z^7+\left(\frac{c^4}{5120}+\frac{1}{7\,340\,032}\right)z^8-\left(\frac{220c^9}{1594\,323}-\frac{11c^5}{139\,968}-\frac{143c}{247\,726\,080}\right)z^9\\&-\left(\frac{286c^{10}}{4782\,969}-\frac{1001c^6}{50\,388\,480}-\frac{2431c^2}{1857\,945\,600}\right)z^{10}+\frac{43c^3}{20\,643\,840}z^{11}\\&+\left(\frac{1547c^{12}}{129\,140\,163}-\frac{2431c^8}{906\,992\,640}+\frac{148\,291c^4}{57\,330\,892\,800}+\frac{1003}{6\,696\,927\,756\,288}\right)z^{12}\Bigg\},\end{aligned} \tag{20}$$

where

$$c = -3\Gamma(\tfrac{3}{4})^4/\pi^2 2^{3/2}.$$

Observe that the first term of the series in Eq. (20) is the same as the asymptotic expression for K given in Eq. (9). The coefficients of the series in Eq. (20) are also in agreement with those for the quantum asymptotic expansion for large quantum numbers n given in Eq. (1.9) of Hioe *et al.*[23] This agreement is consistent with the validity of torus quantization of the BGNF for large n (see Secs. III A and IV B).

Since the direct series, Eq. (3), and the "asymptotic" series, Eq. (20), do not converge at $y = y_0$, and since these series converge only slowly for points near y_0, a third function is required to conveniently represent K at and near y_0. The $[m+1,m]$ Padé approximants, such as the one in Eq. (12), can be used. By using a Padé approximant of suitable order one can *join* to it the asymptotic series at any point $y > y_0$. In practice it is more efficient to construct $[j,j]$ Padé approximants, $P_a[j,j]$, for the asymptotic series and to combine the $P_a[j,j]$ with the $P[m+1,m]$ obtained earlier. The point $y = y_{\text{join}}$ used for joining the two Padé approximants should be in the region of validity of these approximants. We therefore advocate the use of the following expressions as the sum of the BGNF series in the interval $0 \leqslant y \leqslant \infty$:

$$K = K_0\{P[m+1,m]\}^{1/3}, \quad y \leqslant y_{\text{join}}, \tag{21}$$

$$K = (1/gz^2)P_a[j,j], \quad y \geqslant y_{\text{join}}, \tag{22}$$

with appropriate values of m, j, and y_{join}. The coefficients of the [14,14] Padé, $P_a[14,14]$, are given in Table II. Like the $P[m+1,m]$, the $P_a[j,j]$ does not have zeros or poles on the positive real axis. Numerical results obtained by using the two Padé approximants and by their combination are discussed in the following section.

IV. SOME NUMERICAL RESULTS

In this section we discuss the "goodness" of the above-mentioned procedures for the sum of the BGNF of the anharmonic oscillator.

A. Comparison of the periods of the classical motion

While any desired accuracy in K can be achieved by using the Padé approximants of appropriate orders, we restrict our discussion to results that are obtained by joining the $P[14,13]$ and $P_a[14,14]$ at $y = 0.25$. A sensitive test of the accuracy of K is made by evaluating the periods of the system at different energies. In Table III, we compare the periods obtained by (1) evaluating the hypergeometric function of Eq. (14) (and its analytic continuation) and using Eq. (13), (2) by using Eqs. (12) and (13), and (3) by using the expression $K \approx (P_a[14,14])/gz^2$ and Eq. (13). It can be seen from the table that if one uses Eqs. (21) and (22) with $y_{\text{join}} = 0.25$, then the maximum error made in the period is of the order of 10^{-16}. For most practical purposes this error is negligible and hence Eqs. (21) and (22), with $m = 13$, $j = 14$, and $y_{\text{join}} = 0.25$, provide adequate representation of the sum of K for all positive values of y.

The reason for using the two Padé approximants rather than the direct series and the asymptotic series is that the Padé approximants analytically continue the corresponding series. The resulting regions of validity overlap substantially as is illustrated by the data in Table III. Furthermore, the two Padé approximants join smoothly as one can see by evaluating their derivatives at y_{join}.

B. Results of torus quantization

Since the BGNF Hamiltonian is a function of the action K_0, the torus quantization of the system is simple. It is obtained by replacing K_0 (in K) by $n + \frac{1}{2}$ where the integer n is the quantum number. Since the radius of convergence y_0 of the BGNF series is 0.116 162 780 721 1097 the usefulness of the direct series, Eq. (3), is restricted to small values of $y = g(n+\frac{1}{2})$. Our summation of the BGNF series allows the semiclassical quantization of the anharmonic oscillator for *all* values of y.

From Table IV, it is seen that the agreement between the results of the more accurate six-term WKBJ quantum calcu-

TABLE II. Coefficients of the [14,14] Padé approximant, $P_a[14,14] = \{\sum_{i=0}^{14} a_i z^i\}/\{\sum_{i=0}^{14} b_i z^i\}$ of the series gz^2K given in Eq. (20). The normal form K is given by setting $j = 14$ in Eq. (22).

i	a_i	b_i
0	1.000 000 000 000 000 0000	1.000 000 000 000 000 0000
1	2.474 019 639 147 828 5351	2.164 895 567 909 549 4041
2	2.896 604 534 468 449 7231	2.248 755 492 033 467 6660
3	2.135 700 469 762 673 7868	1.485 593 992 001 730 0473
4	1.108 558 558 098 577 1433	0.694 508 929 992 645 2409
5	0.427 741 333 351 820 3117	0.241 674 147 528 744 4151
6	0.126 099 388 725 971 7405	$0.641\,231\,604\,373\,651\,0107 \times 10^{-1}$
7	$0.287\,165\,710\,030\,707\,5826 \times 10^{-1}$	$0.130\,692\,578\,094\,516\,1537 \times 10^{-1}$
8	$0.504\,284\,469\,830\,078\,2695 \times 10^{-2}$	$0.203\,361\,222\,563\,497\,8223 \times 10^{-2}$
9	$0.673\,122\,681\,997\,975\,3551 \times 10^{-3}$	$0.236\,658\,675\,374\,570\,0321 \times 10^{-3}$
10	$0.662\,594\,851\,279\,210\,0445 \times 10^{-4}$	$0.197\,830\,088\,100\,645\,3629 \times 10^{-4}$
11	$0.455\,331\,053\,824\,176\,9842 \times 10^{-5}$	$0.110\,417\,121\,593\,347\,5518 \times 10^{-5}$
12	$0.197\,633\,578\,589\,394\,3311 \times 10^{-6}$	$0.357\,550\,719\,906\,155\,8520 \times 10^{-7}$
13	$0.441\,513\,014\,932\,178\,3171 \times 10^{-8}$	$0.493\,327\,250\,295\,914\,5830 \times 10^{-9}$
14	$0.309\,342\,718\,650\,039\,6539 \times 10^{-10}$	$0.115\,539\,735\,806\,416\,7831 \times 10^{-11}$

TABLE III. Comparison of the periods of the anharmonic oscillator. T_h, T_p, and T_a represent, respectively, the periods obtained by (1) evaluating the hypergeometric function of Eq. (14) (and its analytic continuation) and using Eq. (13), (2) using Eqs. (12) and (13), and (3) using the expression $K \approx P_a[14,14]/gz^2$ and Eq. (13). The last three columns report the magnitudes of the differences identified by the respective column headings. They illustrate the extent to which the Padé approximants have analytically continued the direct and asymptotic series. Because of the large region of overlap, there is considerable freedom in choosing y_{join}. An obvious choice from this table is $y_{\text{join}} = 0.25$. The coefficients required to evaluate T_p and T_a can be found in Tables I and II.

gK_0	T_h	$\lvert T_h - T_p \rvert$	$\lvert T_h - T_a \rvert$	$\lvert T_p - T_a \rvert$
0.10	5.578 514 051 266 051 5780	0.1273×10^{-19}	0.1081×10^{-10}	0.1081×10^{-10}
0.15	5.336 345 803 238 494 1227	0.2003×10^{-19}	0.1219×10^{-12}	0.1219×10^{-12}
0.20	5.135 845 449 401 070 0175	0.1245×10^{-17}	0.3617×10^{-14}	0.3616×10^{-14}
0.25	4.965 470 247 391 742 1306	0.6106×10^{-16}	0.1991×10^{-15}	0.1380×10^{-15}
0.30	4.817 834 889 177 143 4982	0.1124×10^{-14}	0.1662×10^{-16}	0.1107×10^{-14}
0.35	4.687 936 728 690 030 8494	0.1181×10^{-13}	0.2043×10^{-17}	0.1181×10^{-13}
0.40	4.572 235 301 409 713 3601	0.8139×10^{-13}	0.4506×10^{-18}	0.8139×10^{-13}
0.45	4.468 136 302 124 691 6946	0.4109×10^{-12}	0.2213×10^{-18}	0.4109×10^{-12}
0.50	4.373 684 179 224 986 2070	0.1639×10^{-11}	0.1736×10^{-18}	0.1639×10^{-11}

lations and those from the torus quantization of the BGNF sum improves as n increases for any given g. The differences in behavior of the two sets of energies of our model *integrable* system are due to the inherent difference in the quantization procedures rather than a poor representation of the invariant tori (a situation that is common when a low-order BGNF series is used without appropriate summation).

The torus quantization amounts to the quantization of the classical Hamiltonian $K(K_0)$ by the operator $K(\mathbf{K}_0)$, where $\mathbf{K}_0 = -\frac{1}{2}(d^2/d\xi^2 - \xi^2)$. It preserves the Poisson structure of K_0 and K. Other quantizations also preserve the Poisson structure[6] so one is justified in asking how to write the *correct* Schrödinger equation for this nonrelativistic anharmonic oscillator when the Hamiltonian of the system is given in the normal form $K(K_0)$. Further discussion of the quantization of this normal form will appear elsewhere.

V. SUMMARY

We have presented the BGNF series and its summation for an anharmonic oscillator. We have also demonstrated algebraically, through the use of hypergeometric functions, that the BGNF series is the only series representation of this Hamiltonian system as a function of K_0 which preserves the period of the system. The summation of the BGNF series has permitted us to compare the torus quantization results for this system to its quantum results for all energies. In addi-

TABLE IV. Comparison of the torus quantization of the BGNF with known six-term WKBJ quantum results. (The six-term WKBJ results are more accurate than the torus, or equivalently, the one-term WKBJ results.) The quantum energy level and coupling parameter are given by n and g, respectively. The E_{WKBJ} numbers are obtained by rounding off the numbers given by Kesarwani and Varshni[51]. The E_{BGNF} numbers are computed by substituting $g(n+1/2)$ for K_0 in the appropriate Padé approximant as determined by comparing $g(n+1/2)$ with $y_{\text{join}} = 0.25$. For a given value of g, agreement increases with n, whereas for a given value of n, agreement decreases with g.

n	g	$g(n+1/2)$	E_{WKBJ}	E_{BGNF}
0	0.000 10	0.000 050 0	0.500 037 49	0.500 018 75
	0.100 00	0.050 000 0	0.532 635 89	0.517 577 83
2	0.000 10	0.000 250 0	2.500 487 31	2.500 468 58
	0.100 00	0.250 000 0	2.873 979 63	2.865 477 12
	10.000 0	25.000 000	8.317 639 39	8.272 911 80
	40 000.0	100 000.00	127.501 150	126.795 606
10	0.000 10	0.001 050 0	10.508 275 1	10.508 2565
	0.100 00	1.050 000 0	14.933 262 6	14.929 5411
	10.000 0	105.000 00	54.886 285 4	54.868 905 2
	40 000.0	420 000.00	859.417 218	859.141 872
100	0.000 10	0.010 050 0	101.247 040	101.247 022
	0.100 00	10.050 000	252.448 468	252.447 633
	10.000 0	1 005.000 0	1 103.214 33	1 103.210 48
	40 000.0	4 020 000.0	17 458.896 7	17 458.835 6
1000	0.000 10	0.100 050 0	1 067.121 27	1 067.121 26
	0.100 00	100.050 00	5 147.030 66	5 147.030 48
	10.000 0	10 005.000	23 569.318 5	23 569.317 6
	40 000.0	40 020 000.0	373 891.711	373 891.698

tion, our BGNF series has reduced the dynamical equations of the system to a form suitable for addressing some basic questions of quantizing classical systems.

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Joint linearization instabilities in general relativity

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When Einstein's equations are supplemented by symmetry conditions, linearization instabilities can occur that are not present in either of the two sets of equations. The general conditions for this joint instability are investigated. This is illustrated with an example where both the Einstein equations and the flatness condition have more linearized solutions than exact solutions. In a minisuperspace model the geometrical reason for these instabilities is shown.

I. INTRODUCTION

The validity of the linearized approximation to nonlinear geometrical equations, such as Einstein's equations, has been largely clarified in the past decade.[1] It is appropriate to think of solutions as points in a suitable function space; linearized objects are then members of the corresponding tangent space. If the tangent space defined by the linear approximation to the nonlinear equations is the same as the tangent space to the manifold of solutions, then the equations are called linearization stable. Thus linearization stability near a solution means that the solution manifold is smooth near that point—for each direction defined by a solution of the linearized equations there is a family of exact solutions (a curve on the solution manifold) whose tangent is that direction.

Einstein's equations have been shown to be linearization stable about most globally defined solutions, both for asymptotically flat and for spatially compact manifolds. The exceptions are solutions on compact manifolds with Killing vector symmetries. Here there are quadratic conditions, in addition to the linearized equations. These conditions must be satisfied to assure that there be exact solutions corresponding, in the above sense, to solutions of the linearized equations. These quadratic conditions are of global type, involving integrals over a spacelike Cauchy surface. In any finite local region (with boundary), Einstein's equations are always linearization stable.[2]

However, in a remarkable paper,[3] Geroch and Lindblom have recently shown that in the context in which exact solutions are typically discussed the linearized approximation is not always reliable; in fact they exhibited linearization instabilities that are characterized by *local* second-order conditions (and therefore have nothing to do with the global conditions mentioned above). The context where this occurs involves existence of fixed Killing vectors in all the metrics under consideration. This restriction to symmetric metrics[4] is by itself linearization stable, and hence cannot be solely responsible for the instability they find. The Geroch–Lindblom example exhibits another surprising feature, namely that to linear order *all* solutions of their class are "gauge," i.e., related by diffeomorphism to flat space-time; yet in higher order genuinely curved, nonflat solutions are obtained.

Although Geroch and Lindblom give a satisfactory and instructive explanation of these circumstances, they do not interpret their results in the standard language of linearization stability theory. It is the aim of the present paper to show that both of the surprising features found by Geroch and Lindblom are a result of linearization instability in the usual sense, and to give a geometrical interpretation of this as lack of smoothness in a function space setting. The key to our interpretation of this instability is the observation that two linearization stable equations may not remain stable when imposed *jointly*. For functions of a finite number of variables this is the easily visualized fact that the intersection of two smooth surfaces is not necessarily smooth (Fig. 1). In Sec. II we explore this phenomenon, which for brevity we call "joint instability," and we discuss the second-order conditions that follow if the joint stability criterion is violated. For simplicity the equations are written for the finite-dimensional case, but they can be generalized easily to function spaces.

In Sec. III we consider the joint stability of the vacuum Einstein equations and certain symmetry conditions, as well as joint stability of space-time flatness and symmetry conditions. We find that both systems are jointly unstable. Thus there are more symmetric solutions of the linearized Einstein equations than symmetric exact solutions, which is one of the Geroch–Lindblom results; and there are more linearly flat symmetric metrics than exactly flat symmetric metrics, which is the other Geroch–Lindblom result.

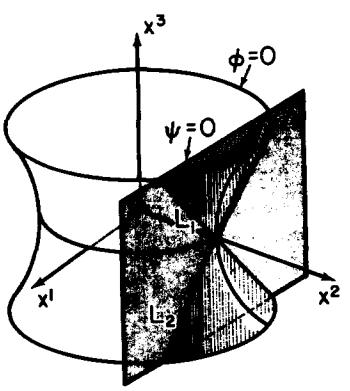

FIG. 1. Simple example of a joint instability. The two surfaces described by Eqs. (4a) and (4b) are everywhere smooth. However, when $a = 1$ their intersection consists of the pair of lines L_1 and L_2. This intersection is not everywhere smooth but has a "conical" singularity at $L_1 \cap L_2$.

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In Sec. IV we construct a finite-dimensional "minisuperspace" of symmetric initial data in which we study the conical structure of the subspace of Einstein solutions, and of flat metrics, which is the geometrical feature associated with these instabilities.

II. JOINT INSTABILITY AND SECOND-ORDER CONDITIONS

We consider the nonlinear equations as a map Φ from a domain D to a range R. The space of solutions S is the subset of D that maps to zero, $\Phi(S)=0$. The linearization of Φ is the differential $d\Phi$ that maps the tangent space at some point of S to the tangent space of the origin of R. Let D be N dimensional, with coordinates x^a, and let S be described by M equations $\phi^i(x^a)=0$ $(a=1,...,N, i=1,...,M)$. If dx^a are coordinates of the tangent space at a point $P\in S$, then the linearized equations about P are

$$d\phi^i=\frac{\partial\phi^i}{\partial x^a}dx^a=0.$$

(Here and in the following all partial derivatives are evaluated at P.) A convenient condition for linearization stability[5] is that $d\Phi$ be a surjective map, that is, if dx^a is allowed to range over the whole tangent space of D then $d\phi^i$ will fill the whole of TR, the tangent space of R.

Suppose Φ and Ψ are equations that can be simultaneously imposed on D, so that they map D to two possibly different ranges R_1, R_2. Suppose further that they are separately linearization stable, hence $d\Phi$ and $d\Psi$ are surjective on TR_1 and TR_2, respectively. Let S_1 and S_2 be the subspaces of D corresponding to the solutions, $\Phi(S_1)=0$, $\Psi(S_2)=0$. Imposing these equations simultaneously defines the intersection $S_1\cap S_2$. We can consider the simultaneous set as a single map $\chi=(\Phi,\Psi)$ that maps D to the direct product $R_1\times R_2$. Then χ is linearization stable—and hence Φ, Ψ are jointly stable—if its differential $d\chi=(d\Phi,d\Psi)$ is surjective on $TR_1\times TR_2$.

If, on the contrary, $d\chi$ is not surjective, there must be a linear relation between $d\Phi$ and $d\Psi$ (since they are linear and separately surjective). That is, there must be one or more covectors $\underset{A}{w}=\left(\underset{A}{u},\underset{A}{v}\right)$ in $T^*R_1\times T^*R_2$ such that, for all $d\chi^a$,

$$\underset{A}{u_i}\frac{\partial\Phi^i}{\partial x^a}dx^a+\underset{A}{v_j}\frac{\partial\Psi^j}{\partial x^a}dx^a=0. \tag{1}$$

As usual in the theory of linearization stability, existence of such $\underset{A}{w}$ allows us to construct second-order conditions on the dx^a. If these conditions are nonempty, there is joint instability. To construct these conditions we evaluate the simultaneous equations $(\Phi,\Psi)=0$ to second order (here d^2 denotes the second derivative, not $d\wedge d$):

$$\begin{aligned}0&=(d^2\Phi^i,d^2\Psi^j)\\&=\left(\frac{\partial^2\Phi^i}{\partial x^a\partial x^b}dx^a\,dx^b+\frac{\partial\Phi^i}{\partial x^a}d^2x^a,\right.\\&\quad\left.\frac{\partial^2\Psi^j}{\partial x^a\partial x^b}dx^a\,dx^b+\frac{\partial\Psi^j}{\partial x^a}d^2x^a\right).\end{aligned} \tag{2}$$

Now we apply the linear relations (1) to find

$$\left(\underset{A}{u_i}\frac{\partial^2\Phi^i}{\partial x^a\partial x^b}+\underset{A}{v_j}\frac{\partial^2\Psi^j}{\partial x^a\partial x^b}\right)dx^a\,dx^b+Q_{ab}\,dx^a\,dx^b=0, \tag{3}$$

that is, one quadratic relation for each of the covectors $\underset{A}{w}$. [These are nonempty, that is, independent of the linearized equations, unless there is a matrix $\underset{A}{L_{ij}}$ such that $Q_{ab}=(\partial\chi^i/\partial x^a)\underset{A}{L_{ij}}(\partial\chi^j/\partial x^b)$. In the latter case, higher-order approximations to the simultaneous equations must be considered to decide about instability.]

A simple example of joint instability is provided by the two surfaces in Euclidean three-space, the hyperboloid

$$\Phi=(x^1)^2+(x^2)^2-(x^3)^2-1=0, \tag{4a}$$

and the plane

$$\Psi=x^1-a=0, \tag{4b}$$

as shown in Fig. 1. For a generic value of a their intersection is smooth, a pair of hyperbolas. However, for $a=1$ it is a pair of intersecting, lines, $x^2=\pm x^3$, hence the two linearization stable equations (4) must be jointly unstable for this value of a. In fact, any point on the intersections satisfies $x^1=a$, $(x^2)^2-(x^3)^2=1-a^2$. For such values of x^2, x^3, the linearization

$$\begin{aligned}dx&=(d\Phi,d\Psi)\\&=(2a\,dx^1+2x^2\,dx^2-2x^3\,dx^3,dx^1),\end{aligned} \tag{5}$$

which maps $\mathbf{R}^3$ to $\mathbf{R}^1\times\mathbf{R}^1$, is surjective whenever x^2 or x^3 differ from zero. However when $a=1$ and $x^2=0=x^3$, we have the linear relation $d\Phi-2d\Psi=0$, which is of the form (1) with $u=1$, $v=-2$. The corresponding quadratic condition (3),

$$2(dx^1)^2+2(dx^2)^2-2(dx^3)^2=0, \tag{6}$$

is nonempty, hence there is a joint instability: the linearized equations for $a=1$ are satisfied by $dx^1=0$ and dx^2, dx^3 arbitrary; but exact simultaneous solutions of (4a) and (4b) exist only for the directions that also satisfy (6).

III. EINSTEIN'S EQUATIONS AND SYMMETRY CONDITIONS

Since it is sufficient, and more convenient, to discuss the stability of the Einstein constraints, we shall assume that the symmetries are spacelike and that the metric has nontrivial time dependence. (This is not essentially different from the case discussed by Geroch and Lindblom, where the metric is independent of x, y, and t but depends on z.) The space-time is described in terms of the initial data on a Cauchy surface,[6] namely the metric g_{ij} of the surface and its conjugate momentum π^{ij} (related to the second fundamental form). The Geroch–Lindblom symmetry condition demands that there be three commuting Killing vectors that are passive, i.e., the same for all metrics. Without loss of generality we can therefore assume that the three spacelike Killing vectors k are the

coordinate directions $\partial/\partial x^i$. The corresponding conditions on the initial data are

$$0 = \Psi(g,\pi) = \begin{cases} \mathcal{L}_k g_{ij}, & (7a) \\ \mathcal{L}_k \pi_{ij}. & (7b) \end{cases}$$

The Einstein constraints are

$$0 = \Phi_1(g,\pi) = \begin{cases} R(g) + \pi_{ij}\pi^{ij} - \frac{1}{2}(\pi_i{}^i)^2, & (8a) \\ \pi^{ij}{}_{|j}, & (8b) \end{cases}$$

and the flatness conditions are the Gauss–Codazzi equations[7]

$$0 = \Phi_2(g,\pi) = \begin{cases} R_{ij}(g) + \pi_{ij}\pi^k{}_j - \frac{1}{2}\pi_{ij}\pi_k{}^k, & (9a) \\ \pi_{ij|k} - \pi_{ik|j} + \frac{1}{2}(g_{ik}\pi_{,j} - g_{ij}\pi_{,k}). & (9b) \end{cases}$$

The linearizations about flat space-time (described by $g_{ij} = \delta_{ij}$, $\pi_{ij} = 0$), written in the usual notation $dg_{ij} = h_{ij}$, $d\pi^{ij} = \omega^{ij}$ take the form

$$d\Psi = \begin{cases} d\Gamma^k_{ij}(h) = \frac{1}{2}(h_{ki,j} + h_{kj,i} - h_{ij,k}), & (10a) \\ \omega^{ij}{}_{,k}, & (10b) \end{cases}$$

$$d\Phi_1 = \begin{cases} dR(h) = d\Gamma^k_{ii,k} - d\Gamma^k_{ik,i}, & (11a) \\ \omega^{ij}{}_{,j}, & (11b) \end{cases}$$

$$d\Phi_2 = \begin{cases} dR_{ij}(h) = d\Gamma^k_{ij,k} - d\Gamma^k_{ik,j}, & (12a) \\ (\omega_{ij,k} - \omega_{ik,j}) + \frac{1}{2}(\delta_{ik}\omega_{,j} - \delta_{ij}\omega_{,k}). & (12b) \end{cases}$$

Note that the equations for h and for ω decouple. Since the exact equations (7b), (8b), (9b) are linear in π, we do not get an instability from the linear relations between (10b), (11b), and (12b). However, the corresponding linear relations between (10a) and (11a) and between (10a) and (12a) do result in second-order equations of the type (3). For example, (11a) is a kind of divergence of (10a) and we have

$$\underset{x}{u} = \delta(x - x'),$$

$$\underset{x}{v^{ij}}{}_k = -\delta^{ij}\delta_{,k}(x - x') + \delta_k{}^j\delta_{,i}(x - x')$$

[where the index A of Eq. (1) corresponds to the continuous index x, the index i to the continuous index x', and the index j to i, j, k, and x'], so that the equation corresponding to (3) obtained from Eqs. (7a) and (8a) becomes

$$d^2R(h,h) + \omega_{ij}\omega^{ij} - (\omega_i{}^i)^2 - d^2\Gamma^k_{ij}(h,h)_{,k} + d^2\Gamma^k_{ik}(h,h)_{,j} = 0$$

$$= \omega_{ij}\omega^{ij} - (\omega_i{}^i)^2. \quad (13)$$

Similarly from Eqs. (10a) and (12a) we get

$$\omega^{ik}\omega_k{}^j - \omega^{ij}\omega_k{}^k = 0. \quad (14)$$

Since the exact equation $\Psi = 0$ actually implies $R_{ij} = 0$ (flat three-space), the exact $\Phi_1 = 0$ and $\Phi_2 = 0$ equations reduce to Eqs. (13) and (14), with ω^{ij} replaced by π^{ij}. It is then easily seen that there are no further conditions on the linearized solutions beyond (13) and (14).

What are the consequences of this joint instability? For Ψ and Φ_2 it means that there are too many linearized symmetric and flat space-time metrics. In fact, once $D\Psi = 0$ is imposed, $d\Phi_2$ always vanishes; that is, any constant h_{ij}, ω^{ij} satisfy the first-order space-time flatness condition. All the corresponding space-time metrics are therefore "gauge," i.e., diffeomorphic (to linear order) to Minkowski space. This is the first surprising feature noted by Geroch and Lindblom.

Similarly, the joint instability of Ψ and Φ_1 means that there are too many linearized symmetric vacuum Einstein metrics; again, all solutions of $d\Psi = 0$ also solve Einstein's equations to linear order. Those corresponding to actual solutions have to satisfy the local second-order condition, Eq. (13). This is the second surprising feature noted by Geroch and Lindblom. [However, their distinction between true and apparent gauge is not represented precisely by our flatness condition (9). For example, all nonvanishing solutions of Eq. (13) would be apparent gauge, but these still include some flat space-times, namely those of Eq. (17) below.]

IV. A MINISUPERSPACE MODEL

The Geroch and Lindblom example that we discussed in Sec. III can be used to construct a minisuperspace[8] that illustrates the conical nature of the solution manifold at points of instability. As initial data we consider only the Euclidean spatial metric δ_{ij} and spatially constant momenta π^{ij}. (We do not consider the corresponding mini-phase space of all spatially constant g_{ij} and π^{ij}, with positive definite g_{ij}, because it has a conical singularity itself at $g_{ij} \to 0$.) These form a six-dimensional space on which the six independent components of π_{ij} are smooth coordinates. We investigate the subspaces $\Phi_1 = 0$ and $\Phi_2 = 0$. Since the symmetry is presupposed, the instability will be exhibited by singularities of these subspaces.

The subspace Σ_1 of solutions of Einstein's equations is described by

$$0 = \Phi_1 = \pi_{ij}\pi^{ij} - (\pi_i{}^i)^2 = \pi^{ij}G_{ijkl}\pi^{kl}, \quad (15)$$

where the DeWitt metric

$$G_{ijkl} = \delta_{ik}\delta_{jl} - \delta_{ij}\delta_{kl} \quad (16)$$

has signature $+ + + + + -$. Therefore Σ_1 is a five-dimensional "light" cone over a four-sphere S^4. [The four-sphere can be obtained by intersecting (15) with the five-plane $\pi_i{}^i = 1$.] The singular point of this cone occurs at $\pi_{ij} = 0$, i.e., at the Minkowski metric for the space-time generated by these initial data. Tangents at that point satisfy the second-order condition (13), but they span the entire six-dimensional space. All directions at the origin that are not on the cone Σ_1 represent unstable solutions of the linearized Einstein constraints.

The subspace Σ_2 representing flat space-time metrics is described by

$$0 = \Phi_2 = \pi^{ik}\pi_k{}^j - \pi_k{}^k\pi^{ij}. \quad (17)$$

The general solution of (17) is

$$\pi^{ij} = v^i v^j, \quad (18)$$

where v^i are the components of an arbitrary spatially constant vector on the initial surface. Therefore Σ_2 is a three-dimensional cone over the two-dimensional surface P described by points π^{ij} of type (18) with v^i a unit vector. Since any such v^i corresponds to a point on the two-sphere S^2, and since v^i and $-v^i$ map via (18) to the same point on P, P is

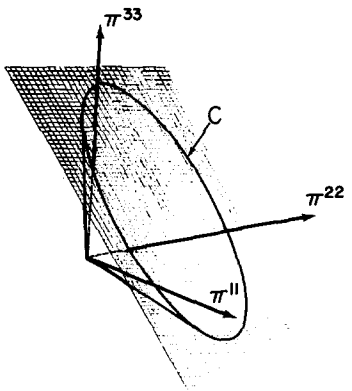

FIG. 2. Minisuperspace of Kasner space-times. The three axes (labeled π^{11}, π^{22}, π^{33}, respectively) represent flat space-times. All other points on the cone represent nonflat Kasner space-times. The plane represents the time coordinate condition $\pi^i_i = \text{const}$. All Kasner solutions satisfying this coordinate condition lie on the circle C.

topologically the projective plane. Since (17) implies (15), Σ_2 is contained in Σ_1 (and $P \subset S^4$). The singular point of Σ_2 is again $\pi^{ij} = 0$, and its tangents again span the entire six-dimensional space. All directions at the origin that are not on Σ_2 represent unstable ("apparently flat") solutions of the linearized flatness conditions.

To recover the Kasner solutions in their usual, diagonal form we reduce the number of minisuperspace dimensions to three by setting

$$\pi^{12} = \pi^{23} = \pi^{13} = 0.$$

The intersection with Σ_1 is a two-dimensional cone; that with Σ_2 consists of three lines (see Fig. 2). Both of these surfaces have a singularity at the origin, illustrating the geometrical reason for the instability in this restricted case. To regain the usual description of the Kasner solutions, we impose the time coordinates condition, $\pi_i{}^i = \text{const}$ (see Ref. 9). The resulting family of solutions form a circle, as shown in the figure. Since these metrics cannot be continuously connected to the Minkowski metric, the geometrical reason for the instability is not apparent with this coordinate condition.

V. CONCLUSIONS

We have seen that two individually linearization stable equations can be jointly unstable when imposed simultaneously. This situation may of course arise in cases other than the example we discussed above. Thus, joint instability may become important in Kaluza–Klein-type theories, where Einstein's equations are supplemented by further conditions.

Our results also have implications for the perturbative approach to quantum gravity. For example, since the Kasner-type perturbation we discussed in first order correspond to gauge transformations, only the phase of the quantum wave functional will vary in first order. Another quantum implication of linearization instability has been pointed out by Moncrief[10]: the operator form of the second-order conditions should be imposed on the wave function of linearized quantum gravity. An analogous procedure has to be followed where there is a joint instability, provided of course that a consistent quantum analog exists of the jointly unstable equations. Similarly, Moncrief conditions arise if there is a classical joint instability, and if the supplementary conditions are solved *before* quantizing (as in the minisuperspace approach).

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[4]In the present discussion metric shall mean metric tensors; that is a description of the geometry in a particular coordinate system. Metrics with a given symmetry form a smooth submanifold of all metrics. In contrast, in the space of geometries, where diffeomorphic metrics are identified, the symmetric geometries lie on strata.

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[6]See, for example, Chap. 21 in C. W. Misner, K. S. Thorne, and J. A. Wheeler, *Gravitation* (Freeman, San Francisco, 1973).

[7]See, for example, N. J. Hicks, *Notes on Differential Geometry* (Van Nostrand, Princeton, NJ, 1965).

[8]This name was originally given to finite-dimensional spaces whose points are symmetric three-geometries [C. W. Misner, in *Magic Without Magic: John Archibald Wheeler*, edited by J. Klauder (Freeman, San Francisco, 1972), pp. 441–473]. Here we consider a finite-dimensional space of symmetric initial data that have not all been identified by diffeomorphisms. It can be regarded as a "minimomentum space" or as a minisuperspace of four-geometries (generated by the Einstein time development equations for *all* initial data, whether solutions of the constraints of not).

[9]The family of metrics used by Geroch and Lindblom,

$$ds^2 = -(\lambda z + 1)^{2p_1}\,dt^2 + (\lambda z + 1)^{2p_2}\,dx^2 + (\lambda z + 1)^{2p_3}\,dy^2 + dz^2,$$

parametrized by λ, p_1, p_2, p_3, also corresponds to points in this minisuperspace if we identify those metrics that are equivalent under a z-translation. Three independent parameters that label these metrics smoothly are $dg_{ii}/dz = 2\lambda p_i$ (related to the diagonal components of π_{ij}).

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The static, cylindrically symmetric strings in general relativity with cosmological constant

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The static, cylindrically symmetric solutions to Einstein's equations with a cosmological term describing cosmic strings are determined. The discussion depends on the sign of the cosmological constant.

I. INTRODUCTION

The static, cylindrically symmetric solution to Einstein's equations describing a cosmic string characterized by a linear mass density μ (for $\mu \neq 1/4G$ in units for which $c=1$, G being the Newton constant) has been recently derived.[1-3] The corresponding space-time is locally flat, but of course it is not globally flat. The singular line source of the field equations, which is the energy-momentum tensor of a cosmic string,[4] is introduced by the existence of a conical singularity[5-7] of the space-time.

The purpose of this paper is to extend these results to the case where the cosmological constant Λ does not vanish. To do this, we shall determine the most general, static, cylindrically symmetric solutions to the field equations

$$R_{\alpha\beta} - \tfrac{1}{2} R g_{\alpha\beta} + \Lambda g_{\alpha\beta} = 0 . \tag{1}$$

The solutions to the field equations (1) depending only on one coordinate have been analyzed already.[8-10] The method can be easily applied in our case. The main result will be to select those that describe a cosmic string and to discuss following the sign of the cosmological constant.

II. THE STATIC CYLINDRICALLY SYMMETRIC METRICS

A static, cylindrically symmetric metric can be written

$$ds^2 = -d\rho^2 - g_2(\rho)dz^2 - g_3(\rho)d\varphi^2 + g_4(\rho)dt^2 , \tag{2}$$

in a coordinate system (t,ρ,z,φ) with $\rho>0$ and $0,\varphi<2\pi$, the hypersurfaces $\varphi=0$ and $\varphi=2\pi$ being identified. The square root of the determinant of metric (2) u is given by

$$u = (g_4 g_2 g_3)^{1/2} . \tag{3}$$

The field equations (1) reduce to the following system of differential equations:

$$\begin{aligned} &((u/g_i)\, g_i')' + 2\Lambda u = 0 , \quad i = 2,3,4 , \\ &\frac{1}{g_2 g_3} g_2' g_3' + \frac{1}{g_3 g_4} g_3' g_4' + \frac{1}{g_4 g_2} g_4' g_2' + 4\Lambda = 0 , \end{aligned} \tag{4}$$

where a prime indicates differentiation with respect to ρ. From system (4), we deduce that u satisfies

$$u'' + 3\Lambda u = 0 , \tag{5}$$

and hence u satisfies

$$u'^2 = -3\Lambda u^2 + K^2 , \tag{6}$$

where K is a strictly positive constant of integration. Taking into account Eq. (4), the first three equations of system (3) can be integrated in the form

$$\frac{1}{g_i} g_i' = \frac{K K_i}{u} + \frac{2u'}{3u} , \quad i = 2,3,4 , \tag{7}$$

where the K_i are three constants of integration. They are not arbitrary; insertion of expressions (7) into the last equation of system (3) yields the following algebraic equations:

$$\begin{aligned} &K_2 + K_3 + K_4 = 0 , \\ &K_2 K_3 + K_3 K_4 + K_4 K_2 = -\tfrac{1}{3} , \end{aligned} \tag{8}$$

which determine the constants K_i in terms of one parameter.

The form of the solution to Eqs. (5) and (6) is dependent on the sign of the cosmological constant. Requiring cylindrically symmetric solutions with respect to the axis $\rho=0$, we must take

$$\begin{aligned} &u(\rho) = [K/(3\Lambda)^{1/2}]\sin[(3\Lambda)^{1/2}\rho] , \quad \text{for } \Lambda>0 , \\ &u(\rho) = [K/(-3\Lambda)^{1/2}]\sinh[(-3\Lambda)^{1/2}\rho] , \quad \text{for } \Lambda<0 . \end{aligned} \tag{9}$$

Substituting u, given by (9), into system (7), the equations can be integrated to give

$$\begin{aligned} &g_i(\rho) = g_i^0 \left\{\tan\left[\frac{(3\Lambda)^{1/2}}{2}\rho\right]\right\}^{K_i} \sin^{2/3}[(3\Lambda)^{1/2}\rho] , \\ &\quad \text{for } \Lambda>0 , \\ &g_i(\rho) = g_i^0 \left\{\tanh\left[\frac{(-3\Lambda)^{1/2}}{2}\rho\right]\right\}^{K_i} \sinh^{2/3}[(-3\Lambda)^{1/2}\rho] , \\ &\quad \text{for } \Lambda<0 , \end{aligned} \tag{10}$$

where the g_i^0 are three constants of integration that have to satisfy

$$g_2^0 g_3^0 g_4^0 = K^2/|3\Lambda| \tag{11}$$

in order to verify relation (3). Moreover we can always give arbitrary values for constants g_4^0 and g_2^0 with the help of an appropriate change of coordinates t and z.

We have now completely determined the general, static metric with cylindrical symmetry (2). They are given by expressions (10) and they depend only on two parameters: the one occurring in the general solution to algebraic equations (8) and the other K. We can calculate straightforwardly the nonvanishing components of the Weyl tensor; we find

$$\begin{aligned} &C^{\rho i}{}_{\rho i} = \frac{K^2}{u^2}\left(\frac{K_i^2}{4} - \frac{2}{9}\right) - \frac{K K_i u'}{6u^2} , \quad i = 2,3,4 , \\ &C^{ij}{}_{ij} = \frac{K^2}{u^2}\left(\frac{K_i K_j}{4} + \frac{1}{9}\right) + \frac{K(K_i + K_j)u'}{6u^2} , \quad i \neq j . \end{aligned} \tag{12}$$

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It may be of interest to note that the Weyl tensor is singular at $\rho = 0$ except for the values of the constants K_i taken as a circular permutation of $-\frac{2}{3}$, $-\frac{2}{3}$, and $\frac{4}{3}$. Moreover for these values it is type D in the Petrov classification.

III. THE STATIC, CYLINDRICALLY SYMMETRIC STRINGS

We now turn to select metrics (2) given by expressions (10), which describe cosmic strings located at $\rho = 0$. We recall that a metric (2) has a conical singularity when in the limit as $\rho \to 0$, it tends to the following form:

$$ds^2 = -d\rho^2 - dz^2 - B^2\rho^2 d\varphi^2 + dt^2, \tag{13}$$

where B is a constant ($B \neq 0$ and $B \neq 1$). Such an asymptotic form (13) induces on the axis a singular part to the source of field equations (1), which is the energy-momentum tensor

$$T_t^t = T_z^z = \frac{1-B}{4G}\frac{\delta(\rho)}{\sqrt{-\tilde{g}}} \quad \text{and} \quad T_\rho^\rho = T_\varphi^\varphi = 0, \tag{14}$$

where $\tilde{g}$ is the determinant of the induced metric on the two-surface, $t = \text{const}$, and $z = \text{const}$. Form (14) of energy-momentum tensor characterizes a static, cylindrically symmetric string of linear mass density μ such that

$$\mu = (1-B)/4G. \tag{15}$$

In order to arrive at the asymptotic form (13) for expressions (10), we must take

$$\begin{aligned} &K_2 = -\tfrac{2}{3}, \quad K_3 = \tfrac{4}{3}, \quad K_4 = -\tfrac{2}{3}, \\ &g_2^0 = 2^{-2/3}, \quad g_3^0 = 2^{4/3}K^2/|3\Lambda|, \quad g_4^0 = 2^{-2/3}. \end{aligned} \tag{16}$$

We remark that this requirement does not fix constant K. Hence metric (2) given by expressions (10) with the choice of constants (16) describes a cosmic string of linear mass density μ given by

$$\mu = (1-K)/4G. \tag{17}$$

IV. CONCLUSION

We have to ask whether the space-times that we have found to describe cosmic strings are regular outside the axis $\rho = 0$. In the case where the cosmological constant is negative, there is no problem. The Weyl tensor is regular everywhere and it is type D in the Petrov classification and moreover it tends to zero for large ρ. On the other hand, in the case where the cosmological constant is positive, it is easy to see from expressions (12) that the invariant $C^{\alpha\beta}{}_{\gamma\delta}C^{\gamma\delta}{}_{\alpha\beta}$ of the Weyl tensor is singular at $\rho = \pi/(3\Lambda)^{1/2}$. Consequently, the geometry of this space-time is singular and such a solution must be rejected.

The above analysis is based on the theory of a conical-type line source. A recent attempt has been made[11] to determine the exterior metric for an extended cosmic string assuming some simple forms of the energy-momentum tensor. Nevertheless, these questions should be reexamined within the theory of a self-interaction scalar field coupled to a gauge field as done by Garfinkle[12] in the case where the cosmological constant vanishes.

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Cartan ideal, prolongation, and Bäcklund transformations for Einstein's equations

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Einstein's equations in the Newman–Penrose formalism for vacuum, vacuum with cosmological constant, and electrovacuum fields are expressed as Cartan ideals. Two different prolongations of these ideals are obtained. These two types of prolonged ideals generalize previous prolongations for vacuum fields to vacuum with cosmological constant and electrovacuum fields. Some Bäcklund transformations are obtained for vacuum, vacuum with cosmological constant, and electrovacuum fields. These Bäcklund transformations include the generalized Kerr–Schild (GKS) transformation, and a two-parameter generalization of the GKS transformation. GKS transformations are studied in detail. Expressions for the transformation of Newman–Penrose quantities are given and algebraic properties are discussed. It is shown that the GKS transformation cannot give algebraically general and asymptotically flat vacuum and electrovacuum space-time metrics.

I. INTRODUCTION

The geometric theory of partial differential equations (PDE's) as found by Cartan,[1–3] besides its own interest, is a useful tool for inverse scattering problems and construction of Bäcklund transformations. The essence of Cartan's approach is to express PDE's as a differential ideal.[4] Then, prolongating this ideal,[5–7] it is possible to obtain "associated equations of the PDE," which are used in solving the original PDE's via inverse scattering methods, or in establishing a correspondence between solutions of the PDE's (i.e., Bäcklund correspondence).

Inverse scattering technique[8] is a well-understood and powerful tool in two-dimensional problems. Extension of this method to higher dimensions is also subject to current interest.[9] The first step in the application of the inverse scattering technique is to find the associated linear equation for the PDE's, i.e., the linear equation whose integrability is guaranteed by the original PDE's. For problems in higher dimensions existence of associated linear equations is not sufficient to solve the PDE's, but they may lead to Bäcklund transformations. The prolongation technique mentioned above can be used to obtain these associated equations. Prolongation was first described by Cartan as a lifting of the ideal representing the PDE's to a fiber bundle, and used to eliminate independent variables. A nontrivial generalization is given by Estabrook and Wahlquist[10] as prolongating the ideal (representing the PDE's) by lifting and adding new generators. These additional generators represent associated equations for the original PDE's.

Applications of inverse scattering to general relativity is practically restricted to space-times admitting symmetries. In fact, space-times admitting two commuting non-null Killing vector fields has been shown to be completely integrable[11,12] and their associated linear equations led to several equivalent Bäcklund transformations.[13–15] The applications of prolongation technique to general relativity starts with Harrison, by the construction of Bäcklund transformations for the Ernst equation.[13] Later work, from Chinea[16] and Gürses,[17] generalize this construction to space-times without symmetries satisfying vacuum Einstein equations: Chinea proposes a linear equation to be useful in inverse scattering (see also Julia[18]). On the other hand, Gürses' approach leads to the construction of Bäcklund transformations,[17,19] which are generalized to Einstein spaces (vacuum with cosmological constant) and electrovacuum fields in the present work.

Prolongation technique, as given by Chinea, Gürses, and Harrison[16,17,20,21] make use of a compact matrix formulation of Einstein's equations obtained from connections in principal bundles. In fact, starting from a null basis for tetrad vectors, the expressions obtained constitute a compact version of the Newman–Penrose (NP) formalism.[22] Expression of Einstein's equations for various (vacuum, vacuum with cosmological constant, electrovacuum) cases in compact form are given in Sec. II.

The formalism described above is used to study Einstein's equations in the framework of Cartan's theory of differential equations: The PDE's in terms of differential forms obtained in Sec. II are used to construct a closed ideal in Sec. III. Then, in Sec. IV prolongated ideals are investigated, and two different prolongations of the ideals constructed in Sec. III are given. One of the prolongations generalizes the equations obtained by Chinea[16] to nonvacuum fields,[19] and the other gives Bäcklund transformations that are discussed in detail in Sec. V. In Sec. V, some Bäcklund transformations are constructed. Construction of the Bäcklund transformation is not sufficient to ensure the existence of new solutions

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since it still remains to solve the associated equations that may well lead (since the system to be solved may be overdetermined) to nontrivial restrictions of the background (i.e., the known solution to start with) or to a trivial solution for the transformation itself. This last step, that is, the solution of associated equations, is presented in detail for the GKS transformation in Sec. VI. The compatibility condition of the GKS transformation for algebraic general backgrounds is found and examples for space-times satisfying these conditions are given. The main feature of this constraint is that vacuum (and in general electrovacuum) backgrounds admitting the GKS transformation cannot be both algebraic general and asymptotically flat,[22,25,26] and since the constraint is invariant under the GKS transformation resulting space-times also will have the same character.[24]

II. EINSTEIN'S EQUATIONS IN THE COMPACT NEWMAN–PENROSE FORMALISM

In this section we will give a compact formulation for the structure equations of a space-time and the Einstein equations. We will essentially express Newman–Penrose (NP) equations[22] in terms of sl(2,C)-valued forms.[27] Then Einstein's equations are obtained simply by equating components of the tracefree Ricci spinor and curvature scalar to corresponding spinorial components of the energy momentum tensor. The crucial point of the formulation is that we have to write these equalities as matrix-valued differential forms that will be suitable for the expression of equations of motion for physical (nongravitational) fields.[17]

In the following we denote by M a space-time manifold with *a Lorentz metric g*. The bundle of orthonormal frames on M is a principal fiber bundle[28,29(a)] with structure group SO(1,3). Then the connection form of M takes its values in the Lie algebra of SO(1,3), and in terms of the canonical form of the frame bundle, structure equations of M can be written in a compact form as

$$de = -\omega \wedge e, \tag{2.1a}$$

$$d\omega = -\omega \wedge \omega + \Omega. \tag{2.1b}$$

In the equations above, e is an $\mathbb{R}^4$ valued one-form. In fact the orthonormal tetrad one-form $e = \{e_k\}$, where $e_k = e_{k\mu}\, dx^\mu$ in a coordinate basis with the metric given by

$$g = e_0 \otimes e_0 - e_1 \otimes e_1 - e_2 \otimes e_2 - e_3 \otimes e_3, \tag{2.2}$$

where $\otimes$ denotes tensor product, and ω and Ω are, respectively, connection and curvature forms taking values in the Lie algebra of SO(1,3). In Eq. (2.1) d is the exterior derivative and $\wedge$ denotes exterior multiplication of corresponding matrices. In the following we will drop the $\wedge$ sign for exterior products, and all multiplications should be understood as appropriate matrix multiplications with exterior products of corresponding forms, unless otherwise stated.

To obtain a compact NP formalism, we will first establish correspondence between an orthonormal frame $\{e_k\}$ and a 2×2 Hermitian matrix whose entries constitute a null frame, then we will give structure equations in terms of this matrix and sl(2,C)-valued forms, and finally we will present transformations of the connection and curvature resulting from the action of SL(2,C) on null frames.

We establish a 1–1 correspondence between the orthonormal frame $\{e_k\}$ and 2×2 Hermitian matrix σ as

$$\sigma = \frac{1}{\sqrt{2}} \sum_{k=0}^{3} (\sigma_k e_k), \tag{2.3a}$$

$$e_k = (1/\sqrt{2})\mathrm{Tr}(\sigma\sigma_k), \quad k = 0,...,3, \tag{2.3b}$$

where the σ_k are Pauli spin matrices, i.e.,

$$\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$
$$\sigma_2 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.4}$$

We then define a null frame $\{l,n,m,\bar{m}\}$ as

$$l = \frac{(e_0 + e_3)}{\sqrt{2}}, \quad n = \frac{(e_0 - e_3)}{\sqrt{2}},$$
$$m = \frac{(e_1 + ie_2)}{\sqrt{2}}, \quad \bar{m} = \frac{(e_1 - ie_2)}{\sqrt{2}}, \tag{2.5}$$

with the metric given by

$$g = l \otimes n + n \otimes l - m \otimes \bar{m} - \bar{m} \otimes m. \tag{2.6}$$

Then Eqs. (2.3a) and (2.5) give an identification of the null frame $\{l,n,m,\bar{m}\}$ with 2×2 Hermitian matrices as

$$\sigma = \begin{pmatrix} l & m \\ \bar{m} & n \end{pmatrix}. \tag{2.7}$$

It can be seen that any other identification of the null frame $\{l,n,m,\bar{m}\}$ with Hermitian 2×2 matrices is similar, either to σ or its complex conjugate $\bar{\sigma}$. We will write all equations in terms of $\tilde{\sigma}$ and $\tilde{\sigma} = \epsilon\sigma\epsilon^\dagger$ (see Ref. 30), where $\epsilon = -i\sigma_2$. That is,

$$\tilde{\sigma} = \begin{pmatrix} n & -\bar{m} \\ -m & l \end{pmatrix}, \quad \bar{\sigma} = \begin{pmatrix} l & \bar{m} \\ m & n \end{pmatrix}. \tag{2.8a}$$

In the following, $\bar{\eta}$ and $\eta^\dagger$ denote complex and Hermitian conjugates of η respectively, and $\tilde{\eta}$ is equal to $\epsilon\eta\epsilon^\dagger$, for any η. Also we have

$$\bar{\Gamma} = -\epsilon\Gamma^\dagger\epsilon^\dagger = -\tilde{\Gamma}^\dagger, \tag{2.8b}$$

$$\bar{\phi} = -\epsilon\phi^\dagger\epsilon^\dagger = -\tilde{\phi}^\dagger. \tag{2.8c}$$

We now give structure equations in terms of $\tilde{\sigma}$ and sl(2,C)-valued connection and curvature forms Γ and R, as

$$d\tilde{\sigma} + \Gamma\tilde{\sigma} - \tilde{\sigma}\Gamma^\dagger = 0, \tag{2.9a}$$

$$d\Gamma + \Gamma\Gamma - R = 0, \tag{2.9b}$$

and we obtain Bianchi identities by taking exterior derivative of Eqs. (2.9a) and (2.9b) as[27]

$$R\tilde{\sigma} + \tilde{\sigma}R^\dagger = 0, \tag{2.10a}$$

$$dR - R\Gamma + \Gamma R = 0, \tag{2.10b}$$

with

$$\Gamma = \begin{pmatrix} \Gamma_0 & \Gamma_2 \\ \Gamma_1 & -\Gamma_0 \end{pmatrix}, \quad R = \begin{pmatrix} R_0 & R_2 \\ R_1 & -R_0 \end{pmatrix}, \tag{2.11}$$

where

$$\Gamma_0 = \gamma l + \epsilon n - \alpha m - \beta\bar{m}, \tag{2.12a}$$

$$\Gamma_1 = -\tau l - \kappa n + \rho m + \sigma\bar{m}, \tag{2.12b}$$

$$\Gamma_2 = \nu l + \pi n - \lambda m - \mu\bar{m}; \tag{2.12c}$$

$$R_0 = (\Lambda - \phi_{11} - \psi_2) ln + \psi_3 lm + \phi_{12} l\bar{m}$$

$$-\phi_{10}nm-\psi_1 n\bar{m}+(\psi_2-\phi_{11}-\Lambda)m\bar{m}, \tag{2.13a}$$

$$R_1=(\psi_1+\phi_{01})ln-(\psi_2+2\Lambda)lm -\phi_{02}l\bar{m}+\phi_{00}nm+\psi_0 n\bar{m}+(\phi_{01}-\psi_1)m\bar{m}, \tag{2.13b}$$

$$R_2=-(\psi_3+\phi_{21})ln+\psi_4 lm+\phi_{22}l\bar{m} -\phi_{20}nm-(\psi_2+2\Lambda)n\bar{m}-(\phi_{21}-\psi_3)m\bar{m}. \tag{2.13c}$$

In Eqs. (2.12), the scalars $\alpha,\beta,\gamma,\lambda,\mu,\nu,\rho,\sigma,\epsilon,\tau,\kappa,\pi$ are NP spin coefficients, and in Eqs. (2.13), $\psi_A\,(A=0,...,4)$, ϕ_{ij} $(i,j=0,...,2)$ are, respectively, components of the Weyl and tracefree Ricci spinor and Λ is the curvature scalar.

We then give transformations of Γ and R corresponding to the SL(2,C) action on null frames. If $S\in$SL(2,C), then the action of S on null frames is given as

$$\tilde{\sigma}\to S\tilde{\sigma}S^{\dagger}. \tag{2.14}$$

This action leaves the metric invariant. The connection Γ and the curvature R transform as

$$\Gamma\to S\Gamma S^{-1}-dSS^{-1}, \tag{2.15a}$$

$$R\to SRS^{-1}. \tag{2.15b}$$

Explicit expressions for Eqs. (2.10), (2.15a), and (2.15b) can be found, for example, in Ref. 31.

Finally we will express Einstein's equations in the NP formalism. They are

$$\phi_{ij}=\tau_{ij},\quad \Lambda=\tau_{\Lambda}, \tag{2.16}$$

where τ_{ij} and τ_{Λ} are the corresponding spinorial components of the energy momentum tensor. Thus to obtain a compact formulation we have to separate tracefree Ricci and curvature scalar components of R by a "compact operation," which is exactly multiplication from the right by $\tilde{\sigma}$. We remark that [Eq. (2.10a)] $R\tilde{\sigma}$ is anti-Hermitian, hence energy momentum tensors will be represented by anti-Hermitian three-form matrices. We give Einstein's equations for vacuum (V), vacuum with cosmological constant ($V+\Lambda$), and electrovacuum (EV) cases in the NP formalism for both component and matrix (compact) form.

(a) Vacuum: In the NP formalism we have $\phi_{ij}=\Lambda=0$. The corresponding equations in compact notation are given as

$$R\tilde{\sigma}=0. \tag{2.17}$$

TABLE I. Einstein's equations for vacuum, vacuum with cosmological constant, and electrovacuum in the Newman–Penrose formalism: component form and compact form.

Vacuum (V)	$\phi_{ij}=0\quad \Lambda=0$	$R\tilde{\sigma}=0$
Vacuum with cosmological constant ($V+\Lambda$)	$\phi_{ij}=0\quad \Lambda=\lambda_0$ λ_0 constant	$R\tilde{\sigma}+\lambda_0\tilde{\sigma}\bar{\tilde{\sigma}}\tilde{\sigma}=0$ λ_0 constant
Electrovacuum (EV)	$\phi_{ij}=2k\phi_i\bar{\phi}_j\quad \Lambda=0$ ϕ_i's given by Eqs. (2.20) Maxwell equations by Eqs. (2.21)	$R\tilde{\sigma}-2k\tilde{\sigma}\phi^{\dagger}\bar{\sigma}\phi\tilde{\sigma}=0$ ϕ given by Eq. (2.24) Maxwell equations by $d(\bar{\sigma}\phi\tilde{\sigma})=0$

(b) Vacuum with cosmological constant (Einstein space): In the NP formalism Einstein equations are $\phi_{ij}=0$ and $\Lambda=\lambda_0$, where λ_0 is a constant. The corresponding equations are given in compact form as

$$R\tilde{\sigma}+\lambda_0\tilde{\sigma}\bar{\tilde{\sigma}}\tilde{\sigma}=0, \tag{2.18}$$

where λ_0 is a constant.

(c) Electrovacuum: In the NP formalism we have

$$\phi_{ij}=2k\phi_i\bar{\phi}_j,\quad \Lambda=0, \tag{2.19}$$

where k is the gravitational constant and the ϕ_i's are given in terms of the Maxwell tensor $F_{\mu\nu}$ as

$$\phi_0=F_{\mu\nu}l^{\mu}m^{\nu}, \tag{2.20a}$$

$$\phi_1=\tfrac{1}{2}F_{\mu\nu}(l^{\mu}n^{\nu}+\bar{m}^{\mu}m^{\nu}), \tag{2.20b}$$

$$\phi_2=F_{\mu\nu}\bar{m}^{\mu}n^{\nu} \tag{2.20c}$$

(recall that $l=l_\mu\,dx^\mu$, $n=n_\mu dx^\mu$, and $m=m_\mu dx^\mu$ in a coordinate basis), and the ϕ_i's satisfy Maxwell's equations:

$$D\phi_1-\bar{\delta}\phi_0=(\pi-2\alpha)\phi_0+2\rho\phi_1-\kappa\phi_2, \tag{2.21a}$$

$$D\phi_2-\bar{\delta}\phi_1=-\lambda\phi_0+2\pi\phi_1+(\rho-2\epsilon)\phi_2, \tag{2.21b}$$

$$\delta\phi_1-\Delta\phi_0=(\mu-2\gamma)\phi_0+2\tau\phi_1-\sigma\phi_2, \tag{2.21c}$$

$$\delta\phi_2-\Delta\phi_1=-\nu\phi_0+2\mu\phi_1+(\tau-2\beta)\phi_2, \tag{2.21d}$$

where $D\eta=l^{\mu}\partial_{\mu}\eta$, $\Delta\eta=n^{\mu}\partial_{\mu}\eta$, and $\delta\eta=m^{\mu}\partial_{\mu}\eta$ for a scalar η. For the purpose of formulating these equations in a compact form, we define the Maxwell two-form as

$$\mathcal{F}=F+i{}^*F=-\phi_1(ln-m\bar{m})-\phi_0 n\bar{m}+\phi_2 lm, \tag{2.22}$$

where $F=F_{\mu\nu}\,dx^{\mu}\,dx^{\nu}$ and ${}^*F$ is the Hodge dual of F, i.e., ${}^*F=\frac{1}{2}\epsilon_{\mu\nu}{}^{\alpha\beta}F_{\alpha\beta}\,dx^{\mu}dx^{\nu}$.

Then the Maxwell equations are simply $d\mathcal{F}=0$. Now we can give electrovacuum Einstein equations in compact form as[30]

$$R\tilde{\sigma}-2k\tilde{\sigma}\phi^{\dagger}\bar{\sigma}\phi\tilde{\sigma}=0, \tag{2.23}$$

where k is the gravitational constant, and

$$\phi=\begin{pmatrix}-\phi_1 & -\phi_2\\ \phi_0 & \phi_1\end{pmatrix}. \tag{2.24}$$

We write the Maxwell two-form as

$$I\mathcal{F}=\bar{\sigma}\phi\tilde{\sigma}, \tag{2.25a}$$

$$I\bar{\mathcal{F}}=-\tilde{\sigma}\phi^{\dagger}\bar{\sigma}, \tag{2.25b}$$

where I is the 2×2 identity matrix and $\bar{\mathcal{F}}$ is the complex conjugate of $\mathcal{F}$. Then Maxwell equations are

$$d(\bar{\sigma}\phi\tilde{\sigma})=0. \tag{2.26}$$

We summarize these results in Table I.

III. CARTAN IDEAL FOR EINSTEIN'S EQUATIONS

Cartan's geometric theory of partial differential equations (PDE's) essentially consists of the description of a PDE as a differential ideal I (equivalently, an exterior differential system) on a manifold N. Then an integral manifold of I will be the pair (M,f), where M is a manifold and f: $M\to N$ is an embedding such that $f^*\alpha_i=0$, for α_i in the ideal I. The differential system is said to be completely integrable if $f(M)$ is a submanifold of N. The terms, integral

submanifold or regular integral manifold, will also be used for such integral manifolds, and the term regular embedding will describe corresponding embeddings.

We recall that[4] systems of PDE's can be represented as systems of homogeneous p-form equations (PDE's in the form of exterior differential equations) by possibly introducing new variables. We describe N to be a manifold with local coordinates consisting of all independent and dependent variables in the PDE's and auxiliary variables introduced in the previous step. Local coordinates of M will consist of independent variables. We then define the forms α_i on N such that their restriction to M gives the PDE's we started with, i.e., for the embedding $f: M \to N, f^*\alpha_i = 0$ gives our PDE's in the form of exterior differential equations. We remark that, if $f^*\alpha_i = 0$, then $f^*(\Sigma_i \xi_i \alpha_i) = 0$ also for forms ξ_i on N. Hence any form in the differential ideal $I = \{\alpha_i\}$ generated by the α_i vanish when restricted to M. Therefore we can conclude that it is rather the ideal generated by the α_i that represents the PDE's.

We note that different sets of generators may represent the same ideal: We define two exterior differential systems $\{\alpha_i\}$ and $\{\alpha_j'\}$ as algebraically equivalent if they generate the same ideal. Then $\{\alpha_i\}$ and $\{\alpha_i'\}$ will represent the same PDE, hence their integral manifolds will be (possibly different) solutions of this PDE.

The closure of an ideal $I = \{\alpha_i\}$ is an ideal $\bar{I} = \{\alpha_i, d\alpha_i\}$ obtained, by adjoining to I, exterior derivatives of its generators. An ideal and its closure have the same integral manifolds since $f^*d\alpha_i = df^*\alpha_i = 0$. An ideal is closed if it is algebraically equivalent to its closure (equivalently if $dI \subset I$). The study of differential systems is concerned mainly with regular integral manifolds of closed ideals.

In this study, our main interest will be the solution generation using Bäcklund transformations and we will not be interested in the existence and complete integrability problems. We only note that, for ideals generated by one-forms (Pfaff systems), the Frobenius theorem states that the system is completely integrable if and only if the corresponding ideal is closed.[4] For higher-order systems we do not have such a complete result,[29(b)] however, the Cartan–Kähler theorem provides (in the real analytic case) a method of construction for integral manifolds starting from lower-dimensional integral manifolds. We will now express the Einstein equations for various sources ($V, V + \Lambda$, EV) as a differential ideal I on a manifold N.

We start by describing local coordinates of M (spacetime manifold to be embedded in N) as x^μ, $\mu = 0,1,2,3$. PDE's in the form of exterior differential equations, representing structure equations, are given by Eqs. (2.9a) and (2.9b), and their integrability conditions, i.e., Bianchi identities are given by (2.10a) and (2.10b). Also Eqs. (2.17), (2.18), and (2.23) represent, respectively, Einstein's equations for $V, V + \Lambda$, and EV fields. Dependent variables consist of the components of the metric (in fact coordinate components of the tetrad frame) of the connection of the curvature, and of the physical fields, for the nonvacuum case. They will constitute, together with x^μ, local coordinates of N. We will construct for $V, V + \Lambda$, and EV, a closed Cartan ideal with generators $\{\alpha_i\}$ such that, for $f: M \to N$ an embedding, $f^*\alpha_i = 0$ gives the corresponding structure and Einstein equations. To be precise, I is two sided, and includes complex conjugates of scalar forms, hence complex conjugates and Hermitian conjugates of matrix forms. We will give for each case ($V, V + \Lambda$, and EV) two algebraic equivalent sets of generators denoted by *generating set A* and *generating set B*.

Generating set A: This generating set defines connection and curvature forms and gives Einstein's equations. We will use this generating set to obtain a prolongation of I that will be used for constructing Bäcklund transformations.[19]

(a) Vacuum: $I = \{\alpha_1, \alpha_2, \alpha_3, \alpha_4\}$, where

$$\alpha_1 = d\tilde{\sigma} + \Gamma\tilde{\sigma} - \tilde{\sigma}\Gamma^\dagger, \tag{3.1}$$

$$\alpha_2 = d\Gamma + \Gamma\Gamma - R, \tag{3.2}$$

$$\alpha_3 = R\tilde{\sigma}, \tag{3.3}$$

$$\alpha_4 = dR - R\Gamma + \Gamma R. \tag{3.4}$$

We note that dim $N = 58$ since we have 10, 24, and 20 variables to describe the metric, connection, and curvature, respectively. Also we remark that $d\alpha_1 = \alpha_3 + \alpha_3^+$ and $d\alpha_2 = \alpha_4$, hence I is closed.

(b) Vacuum with cosmological constant: $I = \{\alpha_1, \alpha_2, \alpha_3, \alpha_4\}$, where α_1, α_2, and α_4 are given by Eqs. (3.1), (3.2), and (3.4), respectively, and

$$\alpha_3 = R\tilde{\sigma} + \lambda_0 \tilde{\sigma}\bar{\tilde{\sigma}}\tilde{\sigma}, \tag{3.5}$$

where λ_0 is a constant. The dim N is still 58. We remark that since $\tilde{\sigma}\bar{\tilde{\sigma}}\tilde{\sigma}$ is anti-Hermitian, $d\alpha_1 \subset I$, and, using Eq. (2.86), we obtain

$$d\bar{\sigma} = \bar{\tilde{\alpha}}_1 + \Gamma^\dagger\bar{\sigma} - \bar{\sigma}\Gamma. \tag{3.6}$$

TABLE II. The *generating set A* and *generating set B* for the Cartan ideal of Einstein's equations for vacuum, vacuum with cosmological constant, and electrovacuum.

	Vacuum	Vacuum with cosmological constant	Electrovacuum
Generating set A	$\alpha_1 = d\tilde{\sigma} + \Gamma\tilde{\sigma} - \tilde{\sigma}\Gamma^\dagger$ $\alpha_2 = d\Gamma + \Gamma\Gamma - R$ $\alpha_3 = R\tilde{\sigma}$ $\alpha_4 = dR - R\Gamma + \Gamma R$	$\alpha_1 = d\tilde{\sigma} + \Gamma\tilde{\sigma} - \tilde{\sigma}\Gamma^\dagger$ $\alpha_2 = d\Gamma + \Gamma\Gamma - R$ $\alpha_3 = R\tilde{\sigma} + \lambda_0\tilde{\sigma}\bar{\tilde{\sigma}}\tilde{\sigma}$ $\alpha_4 = dR - R\Gamma + \Gamma R$	$\alpha_1 = d\tilde{\sigma} + \Gamma\tilde{\sigma} - \tilde{\sigma}\Gamma^\dagger$ $\alpha_2 = d\Gamma + \Gamma\Gamma - R$ $\alpha_3 = R\tilde{\sigma} - 2k\tilde{\sigma}\phi^\dagger\bar{\tilde{\sigma}}\phi\tilde{\sigma}$ $\alpha_4 = dR - R\Gamma + \Gamma R$ $\alpha_5 = d(\bar{\tilde{\sigma}}\phi\tilde{\sigma})$
Generating set B	$\alpha_1 = d\tilde{\sigma} + \Gamma\tilde{\sigma} - \tilde{\sigma}\Gamma^\dagger$ $\alpha_3 = (d\Gamma + \Gamma\Gamma)\tilde{\sigma}$	$\alpha_1 = d\tilde{\sigma} + \Gamma\tilde{\sigma} - \tilde{\sigma}\Gamma^\dagger$ $\alpha_3 = (d\Gamma + \Gamma\Gamma)\tilde{\sigma} + \lambda_0\tilde{\sigma}\bar{\tilde{\sigma}}\tilde{\sigma}$	$\alpha_1 = d\tilde{\sigma} + \Gamma\tilde{\sigma} - \tilde{\sigma}\Gamma^\dagger$ $\alpha_3 = (d\Gamma + \Gamma\Gamma)\tilde{\sigma} - 2k\tilde{\sigma}\phi^\dagger\bar{\tilde{\sigma}}\phi\tilde{\sigma}$ $\alpha_5 = d(\bar{\tilde{\sigma}}\phi\tilde{\sigma})$

Then, it can be checked that $d\alpha_3 \subset I$, hence I is closed.

(c) Electrovacuum: $I = \{\alpha_1,\alpha_2,\alpha_3,\alpha_4,\alpha_5\}$, where α_1,α_2, and α_4 are given by Eqs. (3.1), (3.2), and (3.4), respectively, and

$$\alpha_3 = R\tilde{\sigma} - 2k\tilde{\sigma}\phi^\dagger\bar{\sigma}\phi\tilde{\sigma}, \tag{3.7}$$

$$\alpha_5 = d(\bar{\sigma}\phi\tilde{\sigma}), \tag{3.8}$$

where k is the gravitational constant and ϕ is given by Eq. (2.25), and we note that $\bar{\sigma}\phi\tilde{\sigma}$ is proportional to the identity matrix. For EV fields, $\dim N = 58 + 6 = 64$. Using Eqs. (3.6) and (3.8) it can be checked that $d\alpha_3 \subset I$, hence I is closed.

Generating set B: In this generating set, we omit the definition of the curvature, hence the Bianchi identities, then dimension of N is considerably reduced. This generating set will give a prolongation of I that has been proposed for inverse scattering problems.[16,18,19]

(a) Vacuum: $I = \{\alpha_1,\alpha_3\}$, where α_1 is given by Eq. (3.1) and

$$\alpha_3 = (d\Gamma + \Gamma\Gamma)\tilde{\sigma}, \tag{3.9}$$

than $\dim N = 38$, and again it can be seen that I is closed.

(b) Vacuum with cosmological constant: $I = \{\alpha_1,\alpha_3\}$, where α_1 is given by Eq. (3.1) and

$$\alpha_3 = (d\Gamma + \Gamma\Gamma)\tilde{\sigma} + \lambda_0\tilde{\sigma}\bar{\sigma}\tilde{\sigma}, \tag{3.10}$$

also $\dim N = 38$ and I is closed.

(c) Electrovacuum: $I = \{\alpha_1,\alpha_3,\alpha_5\}$, where α_1 and α_5 are given by Eqs. (3.1) and (3.8) and

$$\alpha_3 = (d\Gamma + \Gamma\Gamma)\tilde{\sigma} - 2k(\tilde{\sigma}\phi^\dagger\bar{\sigma}\phi\tilde{\sigma}). \tag{3.11}$$

In this case, $\dim N = 38 + 6 = 44$, and I is closed.

We present both sets of generators for V, $V + \Lambda$, and EV in Table II.

IV. PROLONGATION OF THE CARTAN IDEAL FOR EINSTEIN'S EQUATIONS

Prolongation of an ideal I in a manifold N is an ideal I' containing I, in a fiber bundle N' over N. If $\pi: N' \to N$ is the projection, we construct I' by lifting the generators $\{\alpha_i\}$ of I to N' and by adding new generators ω_A; that is I' is generated by $\{\pi^*\alpha_i,\omega_A\}$. In this construction the ω_A's are not of the form $\omega_A = d\theta_B$, for $\theta_B \in I'$. Then if $I' = \{\pi^*\alpha_i,\omega_A\}$ is closed, we have a nontrivial prolongation of I, and the PDE we started with is said to have a prolongation structure.[5–7,13,16]

If $(M,f'), f': M \to N'$ is an integral manifold of I', then $f'^*(\pi^*\alpha_i) = 0$ and $f'^*\omega_A = 0$. Therefore $(M,\pi\circ f')$ is an integral manifold of I with additional equations given by $f^*\omega_A = 0$ also solved. Furthermore,[10] for the nontrivial prolonged ideal I' constructed as above, the maximum-dimensional regular integral submanifolds of I and I' are the same. Therefore, if I is a completely integrable system, its prolongation I' is also completely integrable.[4]

In the prolongation process of an ideal representing a PDE, we are interested in finding additional forms that are linear in fiber variables. In these cases, they represent "associated linear equations" for original PDE's. In any case, prolongation forms are useful whenever they represent equations easier to solve than the original PDE's. Although the term "associated linear equation" has a special meaning in inverse scattering problems, we will use the term "associated equations" to designate the equations represented by $f'^*\omega_A = 0$.

In the following sections we will give two different prolongations of the Cartan ideal constructed in Sec. III for V, $V + \Lambda$, and EV field equations. The first construction will give the linear equation proposed to be useful in the inverse scattering approach, the second will lead to Bäcklund transformations.

A. Prolonged ideals using *generating set B*

In this section we construct a prolongation of I using *generating set B* given in Sec. III. In each case (V,$V + A$,EV) associated linear equations are formally the Rarita–Schwinger equations, and fiber variables admit a transformation that leave the associated equations and the ideal invariant. We give the prolonged ideals as follows.

(a) Vacuum: $I' = \{\alpha_1,\alpha_3,\omega\}$, where α_1,α_3 are given by Eqs. (3.1), (3.9), and

$$\omega = \bar{\sigma}(d + \Gamma)\Psi, \tag{4.1}$$

where Ψ is a complex vector one-form. Using Eqs. (3.1), (3.6), and (2.8b), we find

$$d\omega = \tilde{\bar{\alpha}}_1(d\Psi + \Gamma\Psi) + \tilde{\bar{\alpha}}_3^\dagger\Psi + \Gamma^\dagger\omega, \tag{4.2}$$

hence I' is closed.

The transformation

$$\Psi \to \Psi + (d + \Gamma)\varphi, \tag{4.3}$$

where φ is an arbitrary zero-form vector, leaves ω invariant (modulo I).

(b) Vacuum with cosmological constant: $I' = \{\alpha_1,\alpha_3,\omega_1,\omega_2\}$, where α_1,α_3 are given by Eqs. (3.1) and (3.10) and

$$\omega_1 = \bar{\sigma}[(d + \Gamma)\Psi_1 + \mu\tilde{\sigma}\Psi_2], \tag{4.4a}$$

$$\omega_2 = \tilde{\sigma}[(d - \Gamma^\dagger)\Psi_2 + \mu\bar{\sigma}\Psi_1], \tag{4.4b}$$

where $\mu^2 = \lambda_0$ and Ψ_1 and Ψ_2 are one-form vectors. Using Eqs. (3.1), (3.6) and (2.8b), we find

$$d\omega_1 = \tilde{\bar{\alpha}}_1(d\Psi_1 + \Gamma\Psi_1 + \mu\bar{\sigma}\Psi_2) - \mu\tilde{\sigma}\alpha_1\Psi_2 + \tilde{\bar{\alpha}}_3^\dagger\Psi_1 + \Gamma^\dagger\omega_1 + \mu\bar{\sigma}\omega_2, \tag{4.5a}$$

$$d\omega_2 = \alpha_1(d\Psi_2 - \Gamma^\dagger\Psi_2 + \mu\tilde{\sigma}\Psi_1) - \mu\tilde{\sigma}\tilde{\bar{\alpha}}_1\Psi_1 + \alpha_3^\dagger\Psi_2 + \mu\tilde{\sigma}\omega_1 - \Gamma\omega_2, \tag{4.5b}$$

hence I' is closed. It can also be checked that the transformation

$$\Psi_1 \to \Psi_1 + (d + \Gamma)\varphi_1 + \mu\tilde{\sigma}\varphi_2, \tag{4.6a}$$

$$\Psi_2 \to \Psi_2 + (d - \Gamma^\dagger)\varphi_2 + \mu\bar{\sigma}\varphi_1, \tag{4.6b}$$

where φ_1,φ_2 are arbitrary zero-form vectors, leaves the ideal invariant.

(c) Electrovacuum: $I' = \{\alpha_1,\alpha_3,\alpha_5,\omega_1,\omega_2\}$, where α_1,α_3, and α_5 are, respectively, given by Eqs. (3.1), (3.11), and (3.8), and

$$\omega_1 = \bar{\sigma}[(d + \Gamma)\Psi_1 + \mu\phi\tilde{\sigma}\Psi_2], \tag{4.7a}$$

$$\omega_2 = \tilde{\sigma}[(d - \Gamma^\dagger)\Psi_2 + \mu\phi^\dagger\bar{\sigma}\Psi_1], \tag{4.7b}$$

where $\mu^2 = -2k$, Ψ_1 and Ψ_2 are one-form vectors. Using Eqs. (3.1), (3.6), (3.8), (2.8b), and (2.8c), we obtain

$$d\omega_1 = \tilde{\bar{\alpha}}_1(d\Psi_1 + \Gamma\Psi_1) + \tilde{\bar{\alpha}}_3^\dagger\Psi_1 + \mu\alpha_5\Psi_2 + \Gamma^\dagger\omega_1 + \mu\bar{\sigma}\phi\omega_2, \quad (4.8a)$$

$$d\omega_2 = \alpha_1(d\Psi_2 - \Gamma^\dagger\Psi_2) + \alpha_3^\dagger\Psi_2 - \mu\alpha_5^\dagger\Psi_1 + \mu\tilde{\sigma}\phi^\dagger\omega_1 - \Gamma\omega_2, \quad (4.8b)$$

hence I' is a closed ideal. The transformation

$$\Psi_1 \to \Psi_1 + (d+\Gamma)\varphi_1 + \mu\phi\tilde{\sigma}\varphi_2, \quad (4.9a)$$

$$\Psi_2 \to \Psi_2 + (d-\Gamma^\dagger)\varphi_2 + \mu\phi^\dagger\bar{\sigma}\varphi_1 \quad (4.9b)$$

leaves the ideal invariant.

Equation (4.1) was proposed as an associated linear equation for vacuum Einstein equations by Julia[18] and Chinea,[16] and is expected to be useful in finding solutions of Einstein's equations by inverse scattering technique. For space-times admitting symmetries, inverse scattering is reduced to two dimensions, and can be solved,[11–15] but in the general case, application of the inverse scattering technique to general relativity is an open problem. The results of this section are summarized in Table III.

B. Prolonged ideals using *generating set A*

Prolonged ideals described in this section will be used to find Bäcklund transformations. For notational convenience, we introduce the differential operator $\mathbb{D}$ as

$$\mathbb{D}\eta = d\eta + \Gamma\eta + (-1)^p\eta\Gamma^\dagger, \quad (4.10)$$

for any p-form η. We give the prolonged ideals.

(a) Vacuum: $I' = \{\alpha_1,\alpha_2,\alpha_3,\alpha_4,\omega_1,\omega_2\}$, where $\alpha_1, \alpha_2, \alpha_3$, and α_4 are given by Eqs. (3.1), (3.2), (3.3), and (3.4), respectively and

$$\omega_1 = \mathbb{D}\tilde{t} + \omega\tilde{\sigma} + (\omega\tilde{\sigma})^\dagger, \quad (4.11)$$

$$\omega_2 = R\tilde{t} + \mathbb{D}(\omega\tilde{\sigma}), \quad (4.12)$$

where $\tilde{t}$ is a Hermitian and ω is a sl(2,C)-valued (traceless) one-form. We then obtain

$$d\omega_1 = \alpha_2\tilde{t} + \tilde{t}\alpha_2^\dagger - \Gamma\omega_1 - \omega_1\Gamma^\dagger + \omega_2 + \omega_2^\dagger, \quad (4.13)$$

$$d\omega_2 = \alpha_2\omega\tilde{\sigma} + \omega\tilde{\sigma}\alpha_2^\dagger + \alpha_3\omega^\dagger + \omega\alpha_3^\dagger + \alpha_4 t + R\omega_1 - \Gamma\omega_2 + \omega_2\Gamma^\dagger, \quad (4.14)$$

hence I' is closed.

(b) Vacuum with cosmological constant: $I' = \{\alpha_1,\alpha_2,\alpha_3,\alpha_4,\omega_1,\omega_2\}$, where $\alpha_1, \alpha_2, \alpha_3$, and α_4 are given by Eqs. (3.1), (3.2), (3.5), and (3.4), respectively. The first prolongation form ω_1 will be the same as the one given for the vacuum case, i.e., ω_1 is given by Eq. (4.11). The second prolongation form will be obtained by adding a source term to the right-hand side of Eq. (4.12), i.e.,

$$\omega_2 = R\tilde{t} + \mathbb{D}(\omega\tilde{\sigma}) - \chi_1. \quad (4.15)$$

We write χ_1 as

$$\chi_1 = -\mu_0 B_0 - \lambda_0 B_1, \quad (4.16)$$

where λ_0, μ_0 are constants, and

$$B_0 = \tilde{\sigma}\bar{\tilde{\sigma}}\tilde{\sigma}, \quad (4.17)$$

$$B_1 = \tilde{\sigma}\bar{\tilde{\sigma}}\tilde{t} + \tilde{\sigma}\bar{\tilde{t}}\tilde{\sigma} + \tilde{t}\bar{\tilde{\sigma}}\tilde{\sigma}. \quad (4.18)$$

We note that χ_1 is anti-Hermitian, hence Eq. (4.15) expresses that $d\omega_1 \subset I'$, and we need to check only $d\omega_2 \subset I'$. We will use the following forms of Eq. (4.11):

$$d\tilde{t} = \omega_1 - \Gamma\tilde{t} + \tilde{t}\Gamma^\dagger - \omega\tilde{\sigma} + \tilde{\sigma}\omega^\dagger, \quad (4.19)$$

$$d\bar{\tilde{t}} = \bar{\tilde{\omega}}_1 + \Gamma^\dagger\bar{\tilde{t}} - \bar{\tilde{t}}\Gamma + \omega^\dagger\bar{\sigma} - \bar{\sigma}\omega. \quad (4.20)$$

In the following (i.e., for $V+\Lambda$ and EV) the calculation of exterior derivatives will be given, mod I', since complete expressions become increasingly lengthy. We can obtain

$$dB_0 = -\Gamma\tilde{\sigma}\bar{\tilde{\sigma}}\tilde{\sigma} + \tilde{\sigma}\bar{\tilde{\sigma}}\tilde{\sigma}\Gamma^\dagger \quad (\mathrm{mod}\, I').$$

$$dB_1 = -\Gamma(\tilde{\sigma}\bar{\tilde{\sigma}}\tilde{t} + \tilde{\sigma}\bar{\tilde{t}}\tilde{\sigma} + \tilde{t}\bar{\tilde{\sigma}}\tilde{\sigma}) + (\tilde{\sigma}\bar{\tilde{\sigma}}\tilde{t} + \tilde{\sigma}\bar{\tilde{t}}\tilde{\sigma} + \tilde{t}\bar{\tilde{\sigma}}\tilde{\sigma})\Gamma^\dagger - \omega\tilde{\sigma}\bar{\tilde{\sigma}}\tilde{\sigma} + \tilde{\sigma}\bar{\tilde{\sigma}}\tilde{\sigma}\omega^\dagger \quad (\mathrm{mod}\, I'). \quad (4.21)$$

We rewrite them as

$$\mathbb{D}B_0 = 0 \quad (\mathrm{mod}\, I'), \quad (4.22)$$

$$\mathbb{D}B_1 = (1/\lambda_0)[\omega R\tilde{\sigma} - R\tilde{\sigma}\omega^\dagger] \quad (\mathrm{mod}\, I'). \quad (4.23)$$

Therefore,

$$\mathbb{D}\chi_1 = -\omega R\tilde{\sigma} + R\tilde{\sigma}\omega^\dagger \quad (\mathrm{mod}\, I'). \quad (4.24)$$

We now obtain $d\omega_2$ as

$$d\omega_2 = -\mathbb{D}\chi_1 + R\tilde{\sigma}\omega^\dagger - \omega R\tilde{\sigma} \quad (\mathrm{mod}\, I'), \quad (4.25)$$

and Eq. (4.24) implies that $d\omega_2 \subset I'$.

(c) Electrovacuum: $I = \{\alpha_1,\alpha_2,\alpha_3,\alpha_4,\alpha_5,\omega_1,\omega_2,\omega_3,\omega_4\}$, where $\alpha_1,\alpha_2,\alpha_3,\alpha_4$, and ω_1 are given by Eqs. (3.1), (3.2), (3.7), (3.4), (3.8), and (4.11), respectively. We define

$$\omega_2 = R\tilde{t} + \mathbb{D}(\omega\tilde{\sigma}) - \chi_1, \quad (4.26)$$

where

$$\chi_1 = A_0(\phi,\varphi) + A_0(\varphi,\phi) + A_0(\varphi,\varphi) + A_1(\phi,\phi), \quad (4.27)$$

where

$$A_0(u,v) = 2k[\tilde{\sigma}u^\dagger\bar{\tilde{\sigma}}v\tilde{\sigma}], \quad (4.28)$$

$$A_1(u,v) = 2k[\tilde{\sigma}u^\dagger\bar{\tilde{\sigma}}\tilde{v}t + \tilde{\sigma}u^\dagger\bar{\tilde{t}}v\tilde{\sigma} + \tilde{t}u^\dagger\bar{\tilde{\sigma}}v\tilde{\sigma}]. \quad (4.29)$$

In Eqs. (4.28) and (4.29) and throughout Secs. IV and V, u and v replace either ϕ or φ, where ϕ is given by Eq. (2.24) and φ is a SL(2,C)-valued zero-form (whose components are additional field variables).

TABLE III. Prolongation of the Cartan ideal of Einstein's equations using *generating set B* for vacuum, vacuum with cosmological constant, and electrovacuum.

Vacuum	Vacuum with cosmological constant	Electrovacuum
$\alpha_1 = d\tilde{\sigma} + \Gamma\tilde{\sigma} - \tilde{\sigma}\Gamma^\dagger$	$\alpha_1 = d\tilde{\sigma} + \Gamma\tilde{\sigma} - \tilde{\sigma}\Gamma^\dagger$	$\alpha_1 = d\tilde{\sigma} + \Gamma\tilde{\sigma} - \tilde{\sigma}\Gamma^\dagger$
$\alpha_3 = (d\Gamma + \Gamma\Gamma)\tilde{\sigma}$	$\alpha_3 = (d\Gamma + \Gamma\Gamma)\tilde{\sigma} + \lambda_0\tilde{\sigma}\bar{\tilde{\sigma}}\tilde{\sigma}$	$\alpha_3 = (d\Gamma + \Gamma\Gamma)\tilde{\sigma} - 2k\tilde{\sigma}\phi^\dagger\bar{\tilde{\sigma}}\phi\tilde{\sigma}$
		$\alpha_5 = d(\bar{\tilde{\sigma}}\phi\tilde{\sigma})$
$\omega = \bar{\tilde{\sigma}}(d+\Gamma)\Psi$	$\omega_1 = \bar{\tilde{\sigma}}[(d+\Gamma)\Psi_1 + \mu\tilde{\sigma}\Psi_2]$	$\omega_1 = \bar{\tilde{\sigma}}[(d+\Gamma)\Psi_1 + \mu\phi\tilde{\sigma}\Psi_2]$
	$\omega_2 = \tilde{\sigma}[(d-\Gamma^\dagger)\Psi_2 + \mu\bar{\tilde{\sigma}}\Psi_1]$	$\omega_2 = \tilde{\sigma}[(d-\Gamma^\dagger)\Psi_2 + \mu\phi^\dagger\bar{\tilde{\sigma}}\Psi_1]$
	where $\mu^2 = \lambda_0$	where $\mu^2 = -2k$

TABLE IV. Prolongation of the Cartan ideal of Einstein's equations using *generating set A* for vacuum, vacuum with cosmological constant and electrovacuum.

Vacuum	Vacuum with cosmological constant	Electrovacuum
$\alpha_1 = d\tilde{\sigma} + \Gamma\tilde{\sigma} - \tilde{\sigma}\Gamma^\dagger$	$\alpha_1 = d\tilde{\sigma} + \Gamma\tilde{\sigma} - \tilde{\sigma}\Gamma^\dagger$	$\alpha_1 = d\tilde{\sigma} + \Gamma\tilde{\sigma} - \tilde{\sigma}\Gamma^\dagger$
$\alpha_2 = d\Gamma + \Gamma\Gamma - R$	$\alpha_2 = d\Gamma + \Gamma\Gamma - R$	$\alpha_2 = d\Gamma + \Gamma\Gamma - R$
$\alpha_3 = R\tilde{\sigma}$	$\alpha_3 = R\tilde{\sigma} + \lambda_0\tilde{\sigma}\bar{\tilde{\sigma}}\tilde{\sigma}$	$\alpha_3 = R\tilde{\sigma} - 2k\tilde{\sigma}\phi^\dagger\bar{\tilde{\sigma}}\phi\tilde{\sigma}$
$\alpha_4 = dR - R\Gamma + \Gamma R$	$\alpha_4 = dR - R\Gamma + \Gamma R$	$\alpha_4 = dR - R\Gamma + \Gamma R$
		$\alpha_5 = d(\bar{\tilde{\sigma}}\phi\tilde{\sigma})$
$\omega_1 = \mathbb{D}\tilde{t} + \omega\tilde{\sigma} + (\omega\tilde{\sigma})^\dagger$	$\omega_1 = \mathbb{D}\tilde{t} + \omega\tilde{\sigma} + (\omega\tilde{\sigma})^\dagger$	$\omega_1 = \mathbb{D}\tilde{t} + \omega\tilde{\sigma} + (\omega\tilde{\sigma})^\dagger$
$\omega_2 = R\tilde{t} + \mathbb{D}(\omega\tilde{\sigma})$	$\omega_2 = R\tilde{t} + \mathbb{D}(\omega\tilde{\sigma}) - \chi_1$, where	$\omega_2 = R\tilde{t} + \mathbb{D}(\omega\tilde{\sigma}) - \chi_1$, where
	$\chi_1 = -\mu_0 B_0 - \lambda_0 B_1$	$\chi_1 = A_0(\phi,\varphi) + A_0(\varphi,\phi) + A_0(\varphi,\varphi) + A_1(\phi,\phi)$
	$B_0 = \bar{\tilde{\sigma}}\tilde{\sigma}\bar{\tilde{\sigma}}\tilde{\sigma}$	$A_0(u,v) = 2k(\bar{\tilde{\sigma}}u^\dagger\bar{\tilde{\sigma}}v\tilde{\sigma})$
	$B_1 = \bar{\tilde{\sigma}}\sigma\tilde{t} + \bar{\tilde{\sigma}}\bar{\tilde{t}}\tilde{\sigma} + \bar{\tilde{t}}\bar{\tilde{\sigma}}\tilde{\sigma}$	$A_1(u,v) = 2k(\bar{\tilde{\sigma}}u^\dagger\bar{\tilde{\sigma}}v\tilde{t} + \bar{\tilde{\sigma}}u^\dagger\bar{\tilde{t}}v\tilde{\sigma} + \bar{\tilde{t}}u^\dagger\bar{\tilde{\sigma}}v\tilde{\sigma})$
		$\omega_3 = d(\bar{\tilde{\sigma}}\phi\tilde{t} + \bar{\tilde{t}}\phi\tilde{\sigma})$
		$\omega_4 = d(\bar{\tilde{\sigma}}\varphi\tilde{\sigma})$

The remaining prolongation forms are

$$\omega_3 = d(\bar{\tilde{\sigma}}\phi\tilde{t} + \bar{\tilde{t}}\phi\tilde{\sigma}), \tag{4.30}$$

$$\omega_4 = d(\bar{\tilde{\sigma}}\varphi\tilde{\sigma}). \tag{4.31}$$

Since ω_3 and ω_4 are exact and χ_1 is anti-Hermitian, we need to check only if $d\omega_2 \subset I'$. We also note that Eq. (4.26) and (4.15) differ only in the definition of χ_1, therefore $d\omega_2$ will be in I' if (4.25) holds with χ_1 given as in (4.27). To obtain $dA_0(u,v)$ and $dA_1(u,v)$, we use $d(\tilde{a}u^\dagger\bar{\tilde{c}}v\tilde{b}) = \tilde{a}u^\dagger d\bar{\tilde{c}}v\tilde{b} + d(\tilde{a}u^\dagger\bar{\tilde{c}})v\tilde{b} - \tilde{a}u^\dagger d(\bar{\tilde{c}}v\tilde{b})$ (where a, b, and c replace either σ or t) and Eqs. (3.8), (4.30), and (4.31). We obtain

$$d[A_0(u,v)] = 2k[\tilde{\sigma}u^\dagger d\bar{\sigma}\, v\tilde{\sigma}] \pmod{I'}, \tag{4.32}$$

$$d[A_1(\phi,\phi)] = 2k[\tilde{\sigma}\phi^\dagger d\bar{\sigma}\,\phi\tilde{t} + \tilde{\sigma}\phi^\dagger d\bar{t}\,\phi\tilde{\sigma} + t\phi^\dagger d\bar{\sigma}\,\phi\tilde{\sigma}] \pmod{I'}. \tag{4.33}$$

Finally using Eqs. (3.6) and (4.20) (and also the fact that $\bar{\tilde{\sigma}}\phi\tilde{\sigma}$ is proportional to the identity matrix), we write (4.32) and (4.33) as

$$\mathbb{D}A_0(u,v) = 0 \pmod{I'}, \tag{4.34}$$

$$\mathbb{D}A_1(\phi,\phi) = -\omega A_0(\phi,\phi) + A_0(\phi,\phi)\omega^\dagger \pmod{I'}, \tag{4.35}$$

and since $A_0(\phi,\phi) = R\tilde{\sigma} \pmod{I'}$ we have verified that $d\omega_2 \subset I'$.

This completes the second set of prolonged ideals. The results of this section are summarized in Table IV. In the next section we will give a Bäcklund transform using these prolonged ideals.

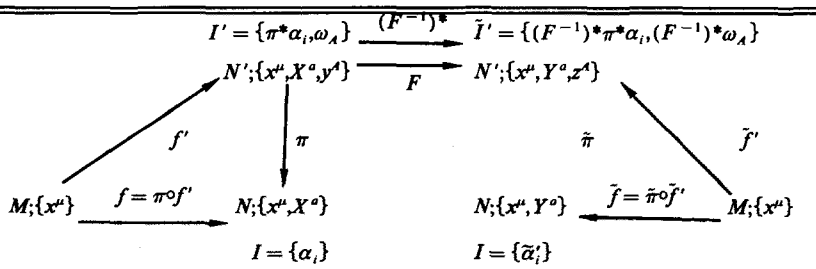
V. BÄCKLUND TRANSFORMATIONS OF EINSTEIN'S EQUATIONS

Bäcklund transformations are basically methods of generating new solutions from known solutions of a PDE. The prolonged ideals that we have constructed in Sec. IV B will be used to find such transformations. We describe the procedure as follows: I is an ideal on N (representing a PDE) generated by $\{\alpha_i\}$ and I' its prolongation on N' (fiber bundle over N, with projection π), with generators $\{\pi^*\alpha_i, \omega_A\}$. We start with a known solution, i.e., an integral submanifold (M,f). Then the construction of I' ensures that (M,f') is an integral submanifold of I' with $f = \pi \circ f'$. We then look for a map $F: N' \to N'$ that induces a diffeomorphism of N, then F induces a (linear) mapping $(F^{-1})^*$ of forms in N. That is $\pi^*\alpha_i$ is mapped to $(F^{-1})^*\pi^*\alpha_i$, as a linear combination of α_i's and ω_A's. If we can choose a special form of F, such that the ideal generated by $\{(F^{-1})^*\pi^*\alpha_i\}$ is algebraically equivalent to I', then $(M, F\circ f')$ will be a new solution for the PDE. Thus F is a Bäcklund transformation relating two solutions of the PDE. If furthermore F can be extended to a diffeomorphism on N' then we can describe $\tilde{I}' = \{(F^{-1})^*\pi^*\alpha_i,\ (F^{-1})^*\omega_A\}$ as prolongated from $(F^{-1})^*\pi^*\alpha' f$. This process is illustrated in Table V.

A. Construction of Bäcklund transformations for Einstein's equations

In order to obtain a Bäcklund transformation, we consider a map F on N', such that $\tilde{\sigma} \to \tilde{\sigma} + \tilde{t}$, $\Gamma \to \Gamma + \omega$,

TABLE V. Bäcklund correspondence for Einstein's equations.



$R \to R + \rho$, $\phi \to \phi + \varphi$. Such a characterization ensures that F induces a diffeomorphism of N'. Then we denote $\tilde{\alpha}_i = (F^{-1})^* \pi^* \alpha_i$, and we can find explicit forms of $\tilde{\alpha}_i$ by simply replacing $\tilde{\sigma}, \Gamma, R, \phi$ in each α_i by their values under F. Therefore

$$\tilde{\alpha}_1 = \alpha_1 + \mathbb{D}\tilde{t} + \omega\tilde{\sigma} + (\omega\tilde{\sigma})^\dagger + (\omega\tilde{t}) + (\omega\tilde{t})^\dagger, \tag{5.1}$$

$$\tilde{\alpha}_2 = \alpha_2 + d\omega + \omega\Gamma + \Gamma\omega + \omega\omega - \rho, \tag{5.2}$$

$$\tilde{\alpha}_4 = \alpha_4 + d\rho - R\omega + \omega R - \rho(\Gamma + \omega) + (\Gamma + \omega)\rho, \tag{5.3}$$

$$\tilde{\alpha}_3 = \alpha_3 + R\tilde{t} + \mathbb{D}(\omega\tilde{\sigma}) + \mathbb{D}(\omega\tilde{t}) + \omega\tilde{\sigma}\omega^\dagger + \omega\tilde{t}\omega^\dagger - \chi_1, \tag{5.4}$$

where

$$\chi_1 = \begin{cases} 0, & \text{for } V, \qquad (5.5) \\ -(\lambda_0 + \mu_0)(\tilde{\sigma} + \tilde{t})(\bar{\sigma} + \bar{\tilde{t}})(\tilde{\sigma} + \tilde{t}) \\ \quad + \lambda_0 \tilde{\sigma}\bar{\tilde{\sigma}}\tilde{\sigma}, & \text{for } V + \Lambda, \qquad (5.6) \\ 2k(\tilde{\sigma} + \tilde{t})(\phi^\dagger + \varphi^\dagger)(\bar{\sigma} + \bar{\tilde{t}})(\phi + \varphi)(\tilde{\sigma} + \tilde{t}) \\ \quad - 2k\tilde{\sigma}\phi^\dagger\bar{\tilde{\sigma}}\phi\tilde{\sigma}, & \text{for EV}; \qquad (5.7) \end{cases}$$

$$\tilde{\alpha}_5 = \alpha_5 + d[(\bar{\sigma} + \bar{\tilde{t}})(\phi + \varphi)(\tilde{\sigma} + \tilde{t})] - d[\bar{\sigma}\phi\tilde{\sigma}]. \tag{5.8}$$

We note that $\tilde{\alpha}_2$ gives the definition of ρ and $\tilde{\alpha}_4$ gives an identity, then, to obtain algebraic equivalence, we have to express $\tilde{\alpha}_1$, $\tilde{\alpha}_3$, and $\tilde{\alpha}_5$ as a sum of α_i's and ω_A's, by equating remaining terms to 0. Comparing Eq. (5.1) with Eqs. (3.1) and (4.11) we obtain

$$\tilde{\alpha}_1 = \alpha_1 + \omega_1, \tag{5.9}$$

$$\omega\tilde{t} + (\omega\tilde{t})^\dagger = 0. \tag{5.10}$$

Now consider three cases.

(a) Vacuum: Comparing Eq. (5.4) with Eqs. (3.3) and (4.12), we have

$$\tilde{\alpha}_3 = \alpha_3 + \omega_2,$$

$$\mathbb{D}(\omega\tilde{t}) + \omega\tilde{\sigma}\omega^\dagger + \omega\tilde{t}\omega^\dagger = 0. \tag{5.11}$$

(b) Vacuum with cosmological constant: Comparing Eqs. (5.4) and (5.6) with Eqs. (3.5) and (4.15), we obtain

$$\tilde{\alpha}_3 = \alpha_3 + \omega_2, \tag{5.12}$$

$$\mathbb{D}(\omega\tilde{t}) + \omega\tilde{\sigma}\omega^\dagger + \omega\tilde{t}\omega^\dagger - \chi_2 = 0, \tag{5.13}$$

where

$$\chi_2 = -\lambda_0(B_2 + B_3) - \mu_0(B_1 + B_2 + B_3), \tag{5.14}$$

with

$$B_1 = \tilde{\sigma}\bar{\sigma}\tilde{t} + \tilde{\sigma}\bar{t}\tilde{\sigma} + \tilde{t}\bar{\sigma}\tilde{\sigma},$$
$$B_2 = \tilde{\sigma}\bar{t}\tilde{t} + \tilde{t}\bar{\sigma}\tilde{t} + \tilde{t}\bar{t}\tilde{\sigma}, \tag{5.15}$$
$$B_3 = \tilde{t}\bar{t}\tilde{t}.$$

(c) Electrovacuum: Comparing Eqs. (5.4) and (5.8) with Eqs. (3.7), (4.26), (3.8), (4.30), and (4.31), we obtain

$$\tilde{\alpha}_3 = \alpha_3 + \omega_2, \tag{5.16a}$$

$$\tilde{\alpha}_5 = \alpha_5 + \omega_3 + \omega_4, \tag{5.16b}$$

$$\mathbb{D}(\omega\tilde{t}) + \omega\tilde{\sigma}\omega^\dagger + \omega\tilde{t}\omega^\dagger - \chi_2 = 0, \tag{5.17a}$$

$$d(\bar{\sigma}\varphi\tilde{t} + \bar{t}\varphi\tilde{\sigma} + \bar{t}(\varphi + \phi)\tilde{t}) = 0, \tag{5.17b}$$

where

$$\chi_2 = \sum_{i=1}^{3} [A_i(\phi,\varphi) + A_i(\varphi,\phi) + A_i(\varphi,\varphi)]$$

$$+ \sum_{i=2}^{3} A_i(\phi,\phi), \tag{5.18}$$

with

$$A_1(u,v) = 2k[\tilde{\sigma}u^\dagger\bar{\sigma}v\tilde{t} + \tilde{\sigma}u^\dagger\bar{t}v\tilde{\sigma} + \tilde{t}u^\dagger\bar{\sigma}v\tilde{\sigma}],$$
$$A_2(u,v) = 2k[\tilde{\sigma}u^\dagger\bar{t}v\tilde{t} + \tilde{t}u^\dagger\bar{\sigma}v\tilde{t} + \tilde{t}u^\dagger\bar{t}v\tilde{\sigma}], \tag{5.19}$$
$$A_3(u,v) = 2k[\tilde{t}u^\dagger\bar{t}v\tilde{t}].$$

To obtain a Bäcklund transform for V, $V + \Lambda$, and EV, we propose to solve the equations

$$\omega\tilde{t} = 0, \tag{5.20}$$

$$\omega\tilde{\sigma}\omega^\dagger - \chi_2 = 0, \tag{5.21}$$

where χ_2 is 0 for V, and is given by Eqs. (5.14) and (5.18) for $V + \Lambda$ and EV, respectively.

B. A method of solution for $\omega\tilde{t} = 0$, $\omega\tilde{\sigma}\omega^\dagger = \chi_2$

We note that, since ω is defined by Eq. (4.12), it is unnecessary to consider it anymore as a fiber coordinate, as long as we solve for the components. Therefore, the first step will be, starting from an arbitrary parametrization of $\tilde{t}$, to solve for the components of ω from Eq. (4.11), i.e., the associated equation $f^*\omega_i = 0$; then to put restrictions either on the background or on the components of $\tilde{t}$ such that $\omega t = 0$ and $\omega\tilde{\sigma}\omega^\dagger = \chi_2$, for the appropriate value of χ_2. The equations for $\tilde{t}$ will be first order, and in general, we will be interested in simple linear equations that are sufficient to solve $\omega\tilde{t} = 0$, $\omega\tilde{\sigma}\omega = \chi_2$. We will give general expressions for ω with $\omega\tilde{t} = 0$. The expression for $\omega\tilde{\sigma}\omega^\dagger$ is cumbersome in the general case, but once ω is found, $\omega\tilde{\sigma}\omega^\dagger$ can be obtained by simple substitutions for each special type of transformation under consideration.

Solution of ω and the constraint equations completes the construction of the Bäcklund transform. But still we may have constraints on the background arising from algebraic or overdetermined equations in ω_2.

We now solve ω from the associated equation $f'^*\omega_1 = 0$, where $\omega_1 = \mathbb{D}\tilde{t} + \omega\tilde{\sigma} - \tilde{\sigma}\omega^\dagger$: Starting with the following parametrization of $\tilde{t}$ and as

$$\tilde{t} = \begin{pmatrix} b_1 & -\bar{c}_1 \\ -c_1 & a_1 \end{pmatrix} l + \begin{pmatrix} b_2 & -\bar{c}_2 \\ -c_2 & a_2 \end{pmatrix} n + \begin{pmatrix} d_2 & -d_4 \\ -d_3 & d_1 \end{pmatrix} m + \begin{pmatrix} \bar{d}_2 & -\bar{d}_3 \\ -\bar{d}_4 & \bar{d}_1 \end{pmatrix} \bar{m}, \tag{5.22a}$$

$$\omega = \begin{pmatrix} \omega_0^1 & \omega_2^1 \\ \omega_1^1 & -\omega_0^1 \end{pmatrix} l + \begin{pmatrix} \omega_0^2 & \omega_2^2 \\ \omega_1^2 & -\omega_0^2 \end{pmatrix} n + \begin{pmatrix} \omega_0^3 & \omega_2^3 \\ \omega_1^3 & -\omega_0^3 \end{pmatrix} m + \begin{pmatrix} \omega_0^4 & \omega_2^4 \\ \omega_1^4 & -\omega_0^4 \end{pmatrix} \bar{m}, \tag{5.22b}$$

we will solve ω from restriction of ω_1 [Eq. (4.11)] on M, i.e.,

$$d\tilde{t} + \Gamma\tilde{t} - \tilde{t}\Gamma^\dagger = -\omega\tilde{\sigma} + \tilde{\sigma}\omega^\dagger. \tag{5.23}$$

We write

$$d\tilde{t} + \Gamma\tilde{t} - \tilde{t}\Gamma^\dagger$$

$$=\begin{pmatrix} A_2 & -\bar{E}_1 \\ -E_1 & A_1 \end{pmatrix} ln + \begin{pmatrix} C_2 & -\bar{E}_3 \\ -E_2 & C_1 \end{pmatrix} lm$$
$$+\begin{pmatrix} \bar{C}_2 & -\bar{E}_2 \\ -E_3 & \bar{C}_1 \end{pmatrix} l\bar{m} + \begin{pmatrix} D_2 & -\bar{E}_5 \\ -E_4 & D_1 \end{pmatrix} nm$$
$$+\begin{pmatrix} \bar{D}_2 & -\bar{E}_4 \\ -E_5 & \bar{D}_1 \end{pmatrix} n\bar{m} + \begin{pmatrix} F_2 & \bar{E}_6 \\ -E_6 & F_1 \end{pmatrix} m\bar{m}, \tag{5.24}$$

and solve for the components of ω as

$$\begin{aligned}
\omega_0^1 &= \tfrac{1}{4}(-2A_2 + E_2 - \bar{E}_2 + F_2),\\
\omega_0^2 &= \tfrac{1}{4}(-2A_1 + E_4 - \bar{E}_4 + F_1),\\
\omega_0^3 &= \tfrac{1}{4}(-C_1 + D_2 + \bar{E}_1 + 2\bar{E}_6),\\
\omega_0^4 &= \tfrac{1}{4}(-\bar{C}_1 + \bar{D}_2 + E_1 - 2E_6),\\
\omega_1^1 &= \tfrac{1}{2}(\bar{C}_1 + \bar{D}_2 + E_1),\\
\omega_1^2 &= \bar{D}_1,\\
\omega_1^3 &= \tfrac{1}{2}(-E_4 - \bar{E}_4 + F_1),\\
\omega_1^4 &= -E_5,\\
\omega_2^1 &= C_2,\\
\omega_2^2 &= \tfrac{1}{2}(C_1 + D_2 - \bar{E}_1),\\
\omega_2^3 &= -\bar{E}_3,\\
\omega_2^4 &= -\tfrac{1}{2}(E_2 + \bar{E}_2 + F_2),
\end{aligned} \tag{5.25}$$

where

$$\begin{aligned}
A_1 &= -Da_1 + \Delta a_2 - 2(\gamma + \bar{\gamma})a_2 - \bar{\kappa}c_1 - \kappa\bar{c}_1 + \bar{\tau}c_2\\
&\quad + \tau\bar{c}_2 - (\tau + \bar{\pi})d_1 - (\bar{\tau} + \pi)\bar{d}_1,\\
A_2 &= -Db_1 + \Delta b_2 - 2(\epsilon + \bar{\epsilon})b_1 + \pi c_1 + \bar{\pi}\bar{c}_1 - \nu c_2\\
&\quad - \bar{\nu}\bar{c}_2 - (\tau + \bar{\pi})d_2 - (\bar{\tau} + \pi)\bar{d}_2,\\
C_1 &= \bar{\delta}a_1 + \Delta d_1 - \bar{\tau}a_1 + \nu a_2 + \bar{\sigma}c_1 + \rho c_1\\
&\quad + (\bar{\mu} - 2\bar{\gamma})d_1 + \lambda\bar{d}_1 + (\tau + \bar{\tau})d_4,\\
C_2 &= \bar{\delta}b_1 + \Delta d_2 + [2(\alpha + \bar{\beta}) - \bar{\tau}]b_1 + \nu b_2 - \lambda c_1\\
&\quad - \bar{\mu}\bar{c}_1 + (\bar{\mu} + 2\gamma)d_2 + \lambda\bar{d}_2 - \nu d_3 - \bar{\nu}d_4,\\
D_1 &= \bar{\delta}a_2 + Dd_1 - \bar{\kappa}a_1 + [-2(\alpha + \bar{\beta}) + \pi]a_2 + \bar{\sigma}c_2\\
&\quad + \rho\bar{c}_2 - (2\bar{\epsilon} + \rho)d_1 + \bar{\sigma}\bar{d}_1 + \bar{\kappa}d_3 + \kappa d_4,\\
D_2 &= \bar{\delta}b_2 + Dd_2 - \bar{\kappa}b_1 + \pi b_2 - \lambda c_2 - \bar{\mu}\bar{c}_2\\
&\quad + (2\epsilon - \rho)d_2 - \bar{\sigma}\bar{d}_2 - \pi d_3 - \bar{\pi}d_4,\\
E_1 &= -Dc_1 + \Delta c_2 + \bar{\pi}a_1 - \bar{\nu}a_2 - \kappa b_1 + \tau b_2\\
&\quad - 2\bar{\epsilon}c_1 - 2\gamma c_2 - (\tau + \bar{\pi})d_3 - (\bar{\tau} + \pi)\bar{d}_4,\\
E_2 &= \bar{\delta}c_1 + \Delta d_3 - \bar{\mu}a_1 + \rho b_1 + (2\bar{\beta} - \bar{\tau})c_1\\
&\quad + \nu c_2 - \bar{\nu}d_1 + \tau d_2 + \bar{\mu}d_3 + \lambda\bar{d}_4,\\
E_3 &= \delta c_1 + \Delta\bar{d}_4 - \bar{\lambda}a_1 + \sigma b_1 + (2\bar{\alpha} - \tau)c_1 + \bar{\nu}c_2\\
&\quad - \bar{\nu}\bar{d}_1 + \tau\bar{d}_2 + \bar{\lambda}d_3 + [\mu + 2(\bar{\gamma} - \gamma)]\bar{d}_4,\\
E_4 &= \bar{\delta}c_2 + Dd_3 - \bar{\mu}a_2 + \rho b_2 + (-2\alpha + \pi)c_2\\
&\quad - \bar{\pi}d_1 + \kappa d_2 - \rho d_3 - \bar{\sigma}\bar{d}_4 - c_1\bar{\kappa},\\
E_5 &= \delta c_2 + D\bar{d}_4 - \bar{\lambda}a_2 + \sigma b_2 + (-2\beta + \bar{\pi})c_2 - \bar{\pi}\bar{d}_1\\
&\quad + \kappa\bar{d}_2 - \sigma d_3 + [2(\bar{\epsilon} - \epsilon) - \bar{\rho}]\bar{d}_4 - c_1\kappa,
\end{aligned} \tag{5.26}$$

$$\begin{aligned}
E_6 &= \delta d_3 - \bar{\delta}\bar{d}_4 + (\rho - \bar{\rho})c_1 + (\mu - \bar{\mu})c_2 - \bar{\lambda}d_1\\
&\quad + \bar{\mu}\bar{d}_1 + \sigma d_2 - \rho\bar{d}_2 + 2(\alpha - \bar{\beta})\bar{d}_4,\\
F_1 &= \delta d_1 - \bar{\delta}\bar{d}_1 + (\rho - \bar{\rho})a_1 + (\mu - \bar{\mu})a_2 - 2\bar{\alpha}d_1\\
&\quad + 2\alpha\bar{d}_1 + \bar{\rho}d_3 - \rho\bar{d}_3 + \sigma d_4 - \bar{\sigma}\bar{d}_4,\\
F_2 &= \delta d_2 - \bar{\delta}\bar{d}_2 + (\rho - \bar{\rho})b_1 + (\mu - \bar{\mu})b_2 + 2\beta d_2\\
&\quad - 2\bar{\beta}\bar{d}_2 - \mu d_3 + \bar{\mu}\bar{d}_3 - \bar{\lambda}d_4 + \lambda\bar{d}_4.
\end{aligned}$$

We then write

$$\tilde{\omega t} = \begin{pmatrix} -N & Q \\ P & -M \end{pmatrix},$$

where

$$\begin{aligned}
M &= [\omega_0^1 a_2 + \omega_1^1\bar{c}_2 - \omega_0^2 a_1 - \omega_1^2\bar{c}_1]ln\\
&\quad + [\omega_0^1 d_1 + \omega_1^1 d_4 - \omega_0^3 a_1 - \omega_1^3\bar{c}_1]lm\\
&\quad + [\omega_0^1\bar{d}_1 + \omega_1^1\bar{d}_3 - \omega_0^4 a_1 - \omega_1^4\bar{c}_1]l\bar{m}\\
&\quad + [\omega_0^2 d_1 + \omega_1^2 d_4 - \omega_0^3 a_2 - \omega_1^3\bar{c}_2]nm\\
&\quad + [\omega_0^2\bar{d}_1 + \omega_1^2\bar{d}_3 - \omega_0^4 a_2 - \omega_1^4\bar{c}_2]n\bar{m}\\
&\quad + [\omega_0^3\bar{d}_1 + \omega_1^3\bar{d}_3 - \omega_0^4 d_1 - \omega_1^4 d_4]m\bar{m},\\
N &= [\omega_2^1 c_2 - \omega_0^1 b_2 - \omega_2^2 c_1 + \omega_0^2 b_1]ln\\
&\quad + [\omega_2^1 d_3 - \omega_0^1 d_2 - \omega_2^3 c_1 + \omega_0^3 b_1]lm\\
&\quad + [\omega_2^1\bar{d}_4 - \omega_0^1\bar{d}_2 - \omega_2^4 c_1 + \omega_0^4 b_1]l\bar{m}\\
&\quad + [\omega_2^2 d_3 - \omega_0^2 d_2 - \omega_2^3 c_2 + \omega_0^3 b_2]nm\\
&\quad + [\omega_2^2\bar{d}_4 - \omega_0^2\bar{d}_2 - \omega_2^4 c_2 + \omega_0^4 b_2]n\bar{m}\\
&\quad + [\omega_2^3\bar{d}_4 - \omega_0^3\bar{d}_2 - \omega_2^4 d_3 + \omega_0^4 d_2]m\bar{m},\\
P &= [\omega_0^1 c_2 + \omega_1^1 b_2 - \omega_0^2 c_1 - \omega_1^2 b_1]ln\\
&\quad + [\omega_0^1 d_3 + \omega_1^1 d_2 - \omega_0^3 c_1 - \omega_1^3 b_1]lm\\
&\quad + [\omega_0^1\bar{d}_4 + \omega_1^1\bar{d}_2 - \omega_0^4 c_1 - \omega_1^4 b_1]l\bar{m}\\
&\quad + [\omega_0^2 d_3 + \omega_1^2 d_2 - \omega_0^3 c_2 - \omega_1^3 b_2]nm\\
&\quad + [\omega_0^2\bar{d}_4 + \omega_1^2\bar{d}_2 - \omega_0^4 c_2 - \omega_1^4 b_2]n\bar{m}\\
&\quad + [\omega_0^3\bar{d}_4 + \omega_1^3\bar{d}_2 - \omega_0^4 d_3 - \omega_1^4 d_2]m\bar{m},\\
Q &= [\omega_2^1 a_2 - \omega_0^1\bar{c}_2 - \omega_2^2 a_1 - \omega_0^2 c_1]ln\\
&\quad + [\omega_2^1 d_1 - \omega_0^1 d_4 - \omega_2^3 a_1 + \omega_0^3\bar{c}_1]lm\\
&\quad + [\omega_2^1\bar{d}_1 - \omega_0^1\bar{d}_3 - \omega_2^4 a_1 + \omega_0^4\bar{c}_1]l\bar{m}\\
&\quad + [\omega_2^2 d_1 - \omega_0^2 d_4 - \omega_2^3 a_2 + \omega_0^3\bar{c}_2]nm\\
&\quad + [\omega_2^2\bar{d}_1 - \omega_0^2\bar{d}_3 - \omega_2^4 a_2 + \omega_0^4\bar{c}_2]n\bar{m}\\
&\quad + [\omega_2^3\bar{d}_1 - \omega_0^3\bar{d}_3 - \omega_2^4 d_1 + \omega_0^4 d_4]m\bar{m}.
\end{aligned} \tag{5.27}$$

Then, to construct a Bäcklund transformation we start with a parametrization of $\tilde{t}$ as given in Eq. (5.22a), then insert these parameters in Eq. (5.26), and using (5.25) we determine the corresponding parametrization of ω, i.e., we have $\omega = \omega(\tilde{t})$. We then insert these expressions in (5.27) to solve $\tilde{\omega t} = 0$. The next section illustrates this method.

C. Examples for Bäcklund transformations of Einstein's equations

1. Example 1 (generalized Kerr–Schild transformation)

Generalized Kerr–Schild transformations constitute an important example for Bäcklund transformations of Einstein's equations. An extensive review of Kerr–Schild transformations can be found, for example, in Kramer *et al.* (see Ref. 23, Chap. 28). Generalized Kerr–Schild transformations are those with nonflat background, and they will be studied in detail in Sec. VI.

We choose $\tilde{t}$ as

$$\tilde{t}=\begin{pmatrix} Vl & 0 \\ 0 & 0 \end{pmatrix}, \tag{5.28}$$

i.e., we let $l\to l$, $n\to n+Vl$, and $m\to m$. Then from Eq. (5.25), by taking $b_1=V$, we obtain

$$\begin{aligned} \omega_0^1 &= \tfrac{1}{2}[DV+2(\epsilon+\bar{\epsilon})V+(\rho-\bar{\rho})V], \\ \omega_0^1 &= \bar{\delta}V+[2(\alpha+\bar{\beta})-\bar{\tau}]V, \\ \omega_2^3 &= -\bar{\sigma}V, \\ \omega_2^4 &= -\rho V, \end{aligned} \tag{5.29}$$

and we can see that, if $\kappa=0$, then $\omega\tilde{t}=0$, hence Eq. (5.10) is satisfied. Then we give

$$\omega\tilde{\sigma}\omega^{\dagger}=\begin{pmatrix} S & 0 \\ 0 & 0 \end{pmatrix}, \tag{5.30}$$

where

$$\begin{aligned} S=V\{&-\tfrac{1}{2}(\rho+\bar{\rho})DV-(\epsilon+\bar{\epsilon})(\rho+\bar{\rho})V \\ &+\tfrac{1}{2}(\rho^2+\bar{\rho}^2)V-\sigma\bar{\sigma}V\}lm\bar{m}. \end{aligned} \tag{5.31}$$

We solve the remaining constraints for V, $V+\Lambda$, and EV as follows.

(a) Vacuum: We have

$$\omega\tilde{\sigma}\omega^{\dagger}=0. \tag{5.32}$$

Therefore, $\kappa=0$ and

$$\begin{aligned} &-\tfrac{1}{2}(\rho+\bar{\rho})DV-(\epsilon+\bar{\epsilon})(\rho+\bar{\rho})V \\ &+\tfrac{1}{2}(\rho^2+\bar{\rho}^2)V-\sigma\bar{\sigma}V=0 \end{aligned} \tag{5.33}$$

solve the constraints.

(b) Vacuum with cosmological constant: We have

$$\omega\tilde{\sigma}\omega^{\dagger}=\chi_2, \tag{5.34a}$$

where χ_2 is given by Eq. (5.20c). We note that $\tilde{t}a\tilde{t}=\bar{t}a\tilde{t}=\tilde{t}a\bar{t}=\bar{t}a\bar{t}\equiv 0$ for any a, and we obtain, from Eq. (5.14),

$$-\chi_2=3\mu_0 V\begin{pmatrix} lm\bar{m} & 0 \\ 0 & 0 \end{pmatrix}. \tag{5.34b}$$

Hence, using Eq. (5.30), we can see that $\kappa=0$ and

$$\begin{aligned} &-\tfrac{1}{2}(\rho+\bar{\rho})DV-(\epsilon+\bar{\epsilon})(\rho+\bar{\rho})V \\ &+\tfrac{1}{2}(\rho^2+\bar{\rho}^2)V-\sigma\bar{\sigma}V=-3\mu_0 V \end{aligned} \tag{5.35}$$

solve the constraints.

(c) Electrovacuum: The constraints are given by Eqs. (5.27a)–(5.27e). We start with

$$\omega\tilde{\sigma}\omega^{\dagger}=\chi_2, \tag{5.36}$$

where χ_2 is given by Eq. (5.25c). We note that $A_2(\phi,\phi)\equiv 0$. Then

$$A_1(u,v)=2kV\begin{pmatrix} -\bar{u}_1 v_1 lm\bar{m} & 0 \\ 0 & 0 \end{pmatrix} \tag{5.37}$$

and using (5.17b) we have

$$\begin{aligned} &-\tfrac{1}{2}(\rho+\bar{\rho})DV-(\epsilon+\bar{\epsilon})(\rho+\bar{\rho})V \\ &+\tfrac{1}{2}(\rho^2+\bar{\rho}^2)V-\sigma\bar{\sigma}V \\ &+2k(\phi_1\bar{\varphi}_1+\bar{\varphi}_1\phi_1+\bar{\varphi}_1\varphi_1)=0. \end{aligned} \tag{5.38}$$

Then we observe that

$$\bar{\sigma}u\tilde{t}+\bar{t}u\tilde{\sigma}=-u_0 Vl\bar{m}, \tag{5.39}$$

hence we take $\varphi_0=0$ to satisfy Eq. (5.17b). Therefore, $\kappa=\phi_0=\varphi_0=0$ and Eq. (5.38) solve the constraints.

2. Example 2

As a second example of Bäcklund transformations, we take the two-parameter transformation, which includes the GKS as a limit. This example is as follows:

$$\tilde{t}=\begin{pmatrix} V & -\bar{Z} \\ -Z & 0 \end{pmatrix}l, \tag{5.40}$$

i.e., we let $l\to l$, $n\to n+Vl$, and $m\to m+Zl$. For this example, we will construct only the Bäcklund correspondence, the solution of the associated equation will be presented elsewhere. To illustrate the Bäcklund construction process, we give the results in detail. We first set $b_1=V$ and $c_1=Z$. We also take $\kappa=0$. Then from Eq. (5.26), we obtain the nonvanishing terms as

$$\begin{aligned} A_2 &= -DV-2(\epsilon+\bar{\epsilon})V+\pi Z+\bar{\pi}\bar{Z}, \\ C_1 &= \rho\bar{Z}+\bar{\sigma}Z, \\ C_2 &= \bar{\delta}V+(2\alpha+2\bar{\beta}-\bar{\tau})V-\lambda Z-\bar{\mu}\bar{Z}, \\ E_1 &= -DZ-2\bar{\epsilon}Z, \\ E_2 &= \bar{\delta}Z+(2\bar{\beta}-\bar{\tau})Z+\rho V, \\ E_3 &= \delta Z+(2\bar{\alpha}-\tau)Z+\sigma V, \\ E_6 &= (\rho-\bar{\rho})Z. \end{aligned} \tag{5.41}$$

We already have $\omega_1^2=\omega_1^3=\omega_1^4=\omega_0^2=0$. Inserting Eq. (5.41) in Eq. (5.27) we have

$$\begin{aligned} M &= 0, \\ N &= -\omega_2^2 Zln+(-\omega_2^3 Z+\omega_0^3 V)lm \\ &\quad +(-\omega_2^4 Z+\omega_0^1 V)l\bar{m}, \\ P &= (-\omega_0^3 Z)lm+(-\omega_0^4 Z)l\bar{m}, \\ Q &= \omega_0^3\bar{Z}lm+\omega_0^4\bar{Z}l\bar{m}. \end{aligned} \tag{5.42}$$

We solve $\omega\tilde{t}=0$ by taking (for $Z\neq 0$)

$$C_1-\bar{E}_1=E_2=E_3=0,\quad \rho-\bar{\rho}=0. \tag{5.43}$$

Therefore we have (for $Z\neq 0$)

$$D\bar{Z}+(2\epsilon+\rho)\bar{Z}+\bar{\sigma}Z=0, \tag{5.44a}$$

$$\bar{\delta}Z+(2\bar{\beta}-\bar{\tau})Z+\rho V=0, \tag{5.44b}$$

$$\delta Z+(2\bar{\alpha}-\tau)Z+\sigma V=0. \tag{5.44c}$$

Nonvanishing components of ω are

$$\begin{aligned} \omega_0^1 &= \tfrac{1}{2}(DV+2(\epsilon+\bar{\epsilon})V-\pi Z-\bar{\pi}\bar{Z}), \\ \omega_1^1 &= (\bar{\rho}Z+\sigma\bar{Z}), \end{aligned} \tag{5.45}$$

TABLE VI. Construction of Bäcklund correspondence for the examples given in Sec. V C.

	Vacuum	Vacuum with cosmological Constant	Electrovacuum
Example 1 GKS	$\kappa=0$	$\kappa=0$	$\kappa=0, \quad \phi_0=0$
$l\to l$	$-\frac{1}{2}(\rho+\bar{\rho})DV-(\epsilon+\bar{\epsilon})(\rho+\bar{\rho})V$	$-\frac{1}{2}(\rho+\bar{\rho})DV-(\epsilon+\bar{\epsilon})(\rho+\bar{\rho})V$	$-\frac{1}{2}(\rho+\bar{\rho})DV-(\epsilon+\bar{\epsilon})(\rho+\bar{\rho})V$
$n\to n+Vl$	$+\frac{1}{2}(\rho^2+\bar{\rho}^2)V-\sigma\bar{\sigma}V=0$	$+\frac{1}{2}(\rho^2+\bar{\rho}^2)V-\sigma\bar{\sigma}V=-3\mu_0$	$+\frac{1}{2}(\rho^2+\bar{\rho}^2)V-\sigma\bar{\sigma}V$
$m\to m$			$+2k(\phi_1\bar{\varphi}_1+\bar{\varphi}_1\phi_1+\varphi_1\bar{\varphi}_1)=0$
Example 2 $l\to l$	$\kappa=0, \quad \rho-\bar{\rho}-0$	$\kappa=0, \quad \bar{\rho}-\rho=0, \quad \mu_0=0$	
$n\to n+Vl$	$D\bar{Z}+(2\epsilon+\rho)\bar{Z}+\bar{\sigma}Z=0$	$D\bar{Z}+(2\epsilon+\rho)\bar{Z}+\bar{\sigma}Z=0$	
$m\to m+Zl$	$\bar{\delta}Z+(2\bar{\beta}-\bar{\tau})Z+\rho V=0$	$\bar{\delta}Z+(2\bar{\beta}-\bar{\tau})Z+\rho V=0$	
	$\delta Z+(2\bar{\alpha}-\tau)Z+\sigma V=0$	$\delta Z+(2\bar{\alpha}-\tau)Z+\alpha V=0$	

hence $\omega\tilde{\sigma}\omega^{\dagger}\equiv 0$. We note that $\tilde{t}a\bar{\tilde{t}}=\bar{\tilde{t}}a\tilde{t}=\tilde{t}a\tilde{t}=\bar{\tilde{t}}a\bar{\tilde{t}}=0$ for this transformation also with a an arbitrary zero-form matrix. Then for vacuum fields all constraints are satisfied identically, but for vacuum with cosmological constant we also need $\mu_0=0$ to construct a Bäcklund correspondence.

We summarize these results in Table VI.

VI. GENERALIZED KERR–SCHILD TRANSFORMATION

The generalized Kerr–Schild (GKS) transformation was given in Sec. V as an example of Bäcklund transformations of Einstein's equations. We started with the parametrization of $\tilde{t}$ given by Eq. (5.28) and we found that if $\kappa=\phi_0=0$ for the background (known solution) and if $\tilde{t}$ satisfies Eq. (5.33), (5.35), or (5.38) (depending on the source) we have a Bäcklund transformation. To find a new solution we have to solve the associated equations given in Table III for various cases.

As an alternative approach to the study of the GKS transformation, we use the Newman–Penrose (NP) formalism in component form (see Table I). Starting from transformation of the tetrad vectors of the form $l\to\tilde{l}$, $n\to\tilde{n}$, $m\to\tilde{m}$, where

$$\tilde{l}=l, \quad \tilde{n}=n+Vl, \quad \tilde{m}=m, \tag{6.1}$$

it is possible to obtain the change in spin coefficients, components of the tracefree Ricci spinor, Weyl spinor, and scalar curvature in an arbitrary background (without assuming any symmetry or any simplifying choice of the tetrad[24]). By a simple study of these expressions it can be seen that $\kappa=0$ is a linearity requirement for the transformation of the tracefree Ricci spinor and the curvature scalar. Furthermore, it can be seen that Eqs. (5.33) and (5.35) are in fact one of the field equations for V and $V+\Lambda$, similarly Eq. (5.38) is a field equation for EV. Therefore if $\kappa=0$, the solution of the associated equations in compact NP formalism is equivalent to solving the transformation equations in component form. The integrability of the solutions is guaranteed by construction of the prolonged ideal in the compact NP formalism.

In the following we will restrict ourselves to the case $\kappa=\phi_{00}=0$ and give in Sec. VI A a brief review of Kerr–Schild metrics, the transformation of NP quantities, and some algebraic properties that follow. In Sec. VI B we give the mixed component of the Einstein tensor and we also observe that (since $l\mu$ is geodesic) the field equations for the new solution are linear in V. We then consider vacuum to vacuum and vacuum to electrovacuum transformations (in fact, we need only a part of the transformation equations to obtain the following results). The main result is that it is not possible to find algebraically general, asymptotically flat vacuum or electrovacuum metrics by applying the GKS transformation to a vacuum metric. This restriction is due to the fact that field equations are overdetermined and give a constraint on the background.

A. GKS transformation: Review and transformation properties

Kerr–Schild (KS) metrics[32] have a special importance in the theory of general relativity. Einstein field equations constructed from these metrics are equivalent to the linearized field equations with flat background.[33] Most of the well-known metrics are in this class. These are the Schwarzschild, the Reissner–Nördstrom, the Kerr, the Kerr–Newman, the Vaidya, p–p waves, and the de Sitter–Schwarzschild metrics. All twisting metrics in this class are obtained from the nontwisting metrics by a complex translation.[33,34] This is due to the fact that the field equations are Lorentz covariant and linear, hence the complexification generates the twisting solutions. In other words, the field equations are also invariant under complex Lorentz transformations.

The generalized Kerr–Schild (GKS) metrics are those with nonflat background. Until now, the space-times described by these metrics (GKS space-time) were considered only for vacuum[35] and pure radiation[36,37] cases. Xanthopoulos[38] has shown that the vacuum field equations corresponding to the GKS metrics are equivalent to the linearized field equations in the background geometry. Taub[37] was interested in the pure radiation and cosmological solutions and using the GKS metrics he found some new solutions. In all the studies mentioned above the background metric is algebraically special. In this work we make no assumption on the background, and we find that there are in fact algebraic general backgrounds, admitting the GKS transformation. We now give the transformation of NP quantities.

The transformation of the spin coefficient can be either obtained by comparing with ω [Eq. (5.25)] or calculated

directly from the expressions for the derivatives of the tetrad frame (i.e., definition of connection), making use of

$$\tilde{D}=D,\quad \tilde{\Delta}=\Delta-VD,\quad \tilde{\delta}=\delta, \tag{6.2}$$

where (D,Δ,δ) and $(\tilde{D},\tilde{\Delta},\tilde{\delta})$ are derivative operators defined in Sec. II, for background and transformed spaces, respectively. In the following all symbols represent scalar quantities and ˜ over a letter denotes the corresponding variable in the transformed space. We will also denote the background by (M,g) and the transformed space by $(M,\tilde{g})$, where g and $\tilde{g}$ denote the corresponding metrics. We recall that we restrict the background to the case $\kappa=0$, $\phi_{00}=0$, and we give the transformations of spin coefficients as

$$\begin{aligned}
&\tilde{\kappa}=0,\quad \tilde{\sigma}=\sigma,\quad \tilde{\rho}=\rho,\\
&\tilde{\epsilon}=\epsilon,\quad \tilde{\tau}=\tau,\quad \tilde{\pi}=\pi,\\
&\tilde{\lambda}=\lambda+\bar{\sigma}V,\quad \tilde{\mu}=\mu+\rho V,\\
&\tilde{\alpha}=\alpha,\quad \tilde{\beta}=\beta,\\
&\tilde{\gamma}=\gamma+\tfrac{1}{2}(D+2\bar{\epsilon}+\rho-\bar{\rho})V,\\
&\tilde{\nu}=\nu+(\bar{\delta}+2\alpha+2\bar{\beta}-\tau-\pi)V.
\end{aligned} \tag{6.3}$$

In Eq. (6.3) and from now on in this section, $\alpha,\beta,\gamma,\lambda,\mu,\nu,\rho,\sigma,\epsilon,\tau,\kappa,\pi$ will denote the NP spin coefficients.

Then the transformations of the tracefree Ricci spinor, curvature scalar, and Weyl spinor can be obtained from NP equations[22] by direct substitution of Eq. (6.3) and making use of Eq. (6.1) as

$$\tilde{\phi}_{ij}=\phi_{ij}+S_{ij},\quad i,j=0,1,2, \tag{6.4}$$

$$\tilde{\Lambda}=\Lambda+S_{\Lambda}, \tag{6.5}$$

$$\tilde{\psi}_i=\psi_i+S_i,\quad i=0,1,2,3,4, \tag{6.6}$$

where the S_{ij}'s, S_n, and S_i are

$$S_{00}=0, \tag{6.7a}$$

$$S_{01}=0, \tag{6.7b}$$

$$S_{02}=\sigma DV+\psi_0 V+\sigma[2(\epsilon+\bar{\epsilon})+(\rho-\bar{\rho})]V, \tag{6.7c}$$

$$\begin{aligned}
2S_{11}=&\tfrac{1}{2}D^2V+\tfrac{3}{2}(\epsilon+\bar{\epsilon})DV+[D(\epsilon+\bar{\epsilon})\\
&+(\epsilon+\bar{\epsilon})^2+\sigma\bar{\sigma}+\rho\bar{\rho}-\rho^2-\rho^2]V,
\end{aligned} \tag{6.7d}$$

$$\begin{aligned}
6S_{\Lambda}=&-\tfrac{1}{2}D^2V-\tfrac{3}{2}(\epsilon+\bar{\epsilon})DV+(\rho+\bar{\rho})DV\\
&+[-D(\epsilon+\bar{\epsilon})-(\epsilon+\bar{\epsilon})^2\\
&+2(\epsilon+\bar{\epsilon})(\rho+\bar{\rho})+\sigma\bar{\sigma}-\rho\bar{\rho}]V,
\end{aligned} \tag{6.7e}$$

$$\begin{aligned}
S_{12}=&\tfrac{1}{2}\delta(D+2\epsilon+2\bar{\epsilon}+\rho-\rho)V+\sigma\bar{\delta}V\\
&+[\psi_1+2\sigma(\alpha+\bar{\beta})-\sigma\bar{\tau}-\rho\tau\\
&+\tfrac{1}{2}(\bar{\alpha}+\beta-\tau)(D+2\epsilon+2\bar{\epsilon}+\rho-\bar{\rho})]V,
\end{aligned} \tag{6.7f}$$

$$\begin{aligned}
S_{22}=&-\Delta(\rho V)+[(\delta-\tau+\bar{\alpha}+3\beta)\\
&\times(\bar{\delta}+2\alpha+2\bar{\beta}-\bar{\tau})+\psi_2\\
&-\mu(D+2\epsilon+2\bar{\epsilon}+\rho-\bar{\rho})\\
&-\rho(\mu+\gamma+\bar{\gamma})-\bar{\lambda}\bar{\sigma}]V,
\end{aligned} \tag{6.7g}$$

$$S_0=0, \tag{6.8a}$$

$$S_1=0, \tag{6.8b}$$

$$\begin{aligned}
3S_2=&\tfrac{1}{2}(D+\epsilon+\bar{\epsilon}+\rho-\bar{\rho})\\
&\times(D+2\epsilon+2\bar{\epsilon}+3\rho-\bar{\rho})V-2\sigma\bar{\sigma}V,
\end{aligned} \tag{6.8c}$$

$$\begin{aligned}
S_3=&VD\alpha+\tfrac{1}{2}(\bar{\delta}+\bar{\beta}-\bar{\tau})(D+2\bar{\epsilon}+\rho-\bar{\rho})V\\
&+(\rho+\epsilon)(\bar{\delta}+2\alpha+2\bar{\beta}-\bar{\tau}-\pi)V\\
&-(\tau+\beta)\bar{\sigma}V+\tfrac{1}{2}\alpha(D+2\epsilon-\rho-\bar{\rho})V,
\end{aligned} \tag{6.8d}$$

$$\begin{aligned}
S_4=&-\Delta(\bar{\sigma}V)+VD(\lambda+\bar{\sigma}V)\\
&+\bar{\delta}(\bar{\delta}+2\alpha+2\bar{\beta}-\bar{\tau}-\pi)V\\
&-\bar{\sigma}V(\mu+\bar{\mu}+3\gamma-\bar{\gamma})\\
&-(\lambda+\bar{\sigma}V)(D+3\bar{\epsilon}-\epsilon+3\rho-\bar{\rho})V\\
&+(3\bar{\alpha}+\beta+\pi-\bar{\tau})\\
&\times(\bar{\delta}+2\alpha+2\bar{\beta}-\bar{\tau}-\pi)V.
\end{aligned} \tag{6.8e}$$

We now give a few results that can be obtained by a simple inspection of Eqs. (6.1)–(6.8).

(a) The transformation of the tetrad basis [Eq. (6.1)] shows that there is a subgroup of the local Sl(2,C) transformations in the background that also leave the transformed metric $\tilde{g}$ invariant. This subgroup consists of null rotations around l^μ, and boosts in the l^μ-n^μ plane and spatial rotations in the m^μ-$\bar{m}^\mu$ plane.[31] Also it can be seen that only the subgroup consisting of spatial rotations in m^μ-$\bar{m}^\mu$ plane commutes with the GKS transform.

(b) Since l^μ is a geodesic null vector in (M,g) [i.e., $l_{\mu;\nu}l^\nu=0$, where a semicolon denotes the covariant derivative in (M,g)], and since $\kappa=l_{\mu;\nu}m^\mu l^\nu=0$ is invariant under the GKS transformation, l_μ is also a geodesic null vector in $(M,\tilde{g})$ (i.e., $l_{\mu|\nu}l^\nu=0$), where | denotes the covariant derivative in $(M,\tilde{g})$.

(c) If the tetrad frame $\tau^a=(l^\mu,n^\mu,m^\mu,\bar{m}^\mu)$ propagates parallely along l^μ (i.e., $l^\mu\tau^a{}_{\nu;\mu}=0$) in (M,g) we have $\kappa=\epsilon=\pi=0$. From the invariance of these spin coefficients we have that $\tilde{\tau}^a=(\tilde{l}^\mu,\tilde{n}^\mu,\tilde{m}^\mu,\tilde{\bar{m}}^\mu)$ propagates parallely along l^μ in $(M,\tilde{g})$ also (i.e., $l^\mu\tilde{\tau}^a{}_{\nu|\mu}=0$).

(d) The optical scalars σ and ρ belonging to the null congruence with the tangent vector l^μ do not change.

(e) If l_μ is a principal null direction (pnd) of the Weyl tensor of (M,g) then $\psi_0=0$, and since l_μ is also geodesic, we have $\tilde{\psi}_0=0$, thus l_μ is also a pnd of the Weyl tensor in $(M,\tilde{g})$.

(f) If the geodesic null vector l_μ is a pnd of (M,g) with multiplicity 1 (i.e., $\psi_0=0$, $\psi_1\neq 0$, the space-time is called algebraically general), then it is a pnd with multiplicity 1 in $(M,\tilde{g})$ also. If l_μ is a pnd with multiplicity 2 (i.e., $\psi_0=\psi_1=\psi_2\neq 0$, the space-time is called algebraically special), then it is a pnd with multiplicity at least 2 in $(M,\tilde{g})$. In other words, if l_μ is a geodesic null vector and a pnd in (M,g), then $(M,\tilde{g})$ will be algebraically general (special) if and only if (M,g) is algebraically general (special), but in the case (M,g) is algebraically special $(M,\tilde{g})$ need not be of the same type.

B. The field equations

Starting from the expression of the Einstein tensor given as

$$G_{\mu\nu}=2\phi_{22}l_\mu l_\nu+2\phi_{00}n_\mu n_\nu+2\phi_{20}m_\mu m_\nu+2\phi_{02}\bar{m}_\mu\bar{m}_\nu$$

$$+2(\phi_{11}+3\Lambda)(l_\mu n_\nu+n_\mu l_\nu)$$
$$+2(\phi_{11}-3\Lambda)(m_\mu\bar{m}_\nu+\bar{m}_\mu m_\nu)$$
$$-2\phi_{21}(l_\mu m_\nu+m_\mu l_\nu)-2\phi_{12}(l_\mu\bar{m}_\nu+\bar{m}_\mu l_\nu)$$
$$-2\phi_{10}(n_\mu m_\nu+m_\mu n_\nu)-2\phi_{01}(n_\mu\bar{m}_\nu+\bar{m}_\mu n_\nu), \tag{6.9}$$

and using Eqs. (6.4)–(6.8), we obtain for the mixed component of the Einstein tensor

$$\tilde{G}^\mu_\nu = G^\mu_\nu - 2(S_{11}-3S_\Lambda)\delta^\mu_\nu$$
$$+2[S_{22}-V^2(\phi_{00}+S_{00})]l^\mu l_\nu+2S_{00}n^\mu n_\nu$$
$$+2S_{20}m^\mu m_\nu+2S_{02}\bar{m}^\mu\bar{m}_\nu+4S_{11}(l^\mu n_\nu+n^\mu l_\nu)$$
$$-2V(\phi_{00}+S_{00})(l^\mu n_\nu-n^\mu l_\nu)$$
$$-2S_{21}(l^\mu m_\nu+m^\mu l_\nu)$$
$$+2V(\phi_{10}+S_{10})(l^\mu m_\nu-m^\mu l_\nu)$$
$$-2S_{12}(l^\mu\bar{m}_\nu+\bar{m}^\mu l_\nu)$$
$$+2V(\phi_{01}+S_{01})(l^\mu\bar{m}_\nu-\bar{m}^\mu l_\nu)$$
$$-2S_{10}(n^\mu m_\nu+m^\mu n_\nu)-2S_{01}(n^\mu\bar{m}_\nu+\bar{m}^\mu n_\nu). \tag{6.10}$$

Thus it can be seen that when l_μ is geodesic (note that $S_{22}-V^2\phi_{00}$ is linear for $\kappa=0$) and $\phi_{00}=0$, G^μ_ν is a linear functional of V. This is an important property that can be used for various purposes: If the background space-time is specified then the gravitational field equations become linear partial differential equations for V. Another consequence of this property follows: If a solution of the Einstein field equations can be put in the GKS form, i.e., $\tilde{g}_{\mu\nu}=g_{\mu\nu}+2Vl_\mu l_\nu$, where $g_{\mu\nu},V,l_\mu$ are all known and if (M,g) has a cyclic coordinate, then any complex translation generates a new solution of the Einstein field equations. These solutions may or may not be distinct.

Now we shall study the Einstein field equations, first assuming the background space-time is fixed. We recall that the transformation of the NP quantities are given for $\kappa=0$ and $\phi_{00}=0$. Also, for electrovacuum, ϕ_{00} implies $\phi_0=0$, hence $\phi_{01}=\phi_{02}=0$. Since $S_{00}=0$ we have $\tilde{\phi}_0=0$ therefore $S_{01}=S_{02}=0$ (in fact $S_{01}\equiv 0$). Thus, in the cases under consideration, the backgrounds V and EV satisfy $\phi_{00}=\phi_{01}=\phi_{02}=0$ and a first set of transformation equations are given by $S_{02}=S_\Lambda=0$ (since $S_{00}=S_{01}=0$). Also the equations giving the Bäcklund correspondence [Eq. (5.33) for V and Eq. (5.38) for EV] is equivalent to the $S_{11}+3S_\Lambda$ term.

We rewrite the transformation of the tracefree Ricci spinor and curvature scalar for V, $V+\Lambda$, and EV as

$$S_{02}=0, \tag{6.11a}$$
$$6S_\Lambda=0, \tag{6.11b}$$
$$2S_{11}=4k(\phi_1\bar{\varphi}_1+\varphi_1\bar{\phi}_1+\varphi_1\bar{\varphi}_1), \tag{6.11c}$$
$$S_{12}=2k(\phi_1\bar{\varphi}_2+\varphi_1\bar{\phi}_2+\varphi_1\bar{\varphi}_2), \tag{6.11d}$$
$$S_{22}=2k(\phi_2\bar{\varphi}_2+\varphi_2\bar{\phi}_2+\varphi_2\bar{\varphi}_2). \tag{6.11e}$$

From (6.11) it can be seen that the solution of V depends crucially on $\rho+\bar{\rho}$ and σ, and the main compatibility problem is in the solution of DV. For $\sigma=0$, we have a consistent system, and the solution will depend on arbitrary constants only, unless $\rho+\bar{\rho}=0$ (in this case ΔV is not specified and the solution will depend on an arbitrary function). But since $\kappa=0$ and $\phi_{00}=\phi_{01}=\phi_{02}=0$, then $\sigma=0$ implies that background is algebraically special with $\psi_0=\psi_1=0$ (Goldberg–Sachs theorem[23]). Also it can be seen that $\rho+\bar{\rho}=0$ implies $\sigma=0$. In the following we will be interested in algebraic general backgrounds admitting the GKS transformation, hence we will take $\sigma\neq 0$, $\rho+\bar{\rho}\neq 0$. We analyze the solutions for two cases: (i) $S_{11}=0$, and (ii) $S_{11}\neq 0$. The first case includes $V\to V$, $V\to$null EV [$\phi_1=0$ (see Ref. 27)] transformations, and the second represent $V\to$(non-null) EV transformations.

(i) $S_{11}=0$: We solve DV from Eq. (6.11c) as

$$DV=\omega_0 V, \tag{6.12}$$

where

$$\omega_0=(\rho+\bar{\rho})^{-1}[\rho^2+\bar{\rho}^2-2\sigma\bar{\sigma}-2(\rho+\bar{\rho})(\epsilon+\bar{\epsilon})]. \tag{6.13}$$

Then $S_\Lambda=0$ is satisfied, but from $S_{02}=0$, we obtain the following constraint on the background:

$$\psi_0/2\sigma=(\rho+\bar{\rho})^{-1}(\sigma\bar{\sigma}-\rho^2). \tag{6.14}$$

(ii) $S_{11}\neq 0$: We solve DV from Eq. (6.11c). Then using $S_{02}=0$, and $S_\Lambda=0$, we obtain

$$D[(\psi_0/\sigma)+2\rho]$$
$$=[(\psi_0/\sigma)+2\rho]^2+(\epsilon+\bar{\epsilon})[(\psi_0/\sigma)+2\rho]. \tag{6.15}$$

Using Bianchi identities it can be seen that this condition is true whenever $S_{00}=S_{01}=S_{02}=S_0=0$.

Then V is the solution of

$$DV=\omega_0 V+u_0, \tag{6.16}$$

where ω_0 is given by Eq. (6.13), and

$$u_0=4k(\phi_1\bar{\varphi}_1+\bar{\varphi}_1\phi_1+\varphi_1\bar{\varphi}_1). \tag{6.17}$$

The constraints (6.14) and (6.15) are satisfied in the cylindrical class of metrics described by Newman and Tamburino[39] and in stationary vacuum space-times discussed by Kota and Perjés.[40]

We now give expressions for δV and ΔV. From Eq. (6.11d) we obtain

$$[(\rho^2-\sigma\bar{\sigma})/(\rho+\bar{\rho})]\delta V+\sigma\bar{\sigma}V+\Omega V=S_{12}, \tag{6.18}$$

where

$$\Omega=\psi_1+(\delta+\bar{\alpha}+\beta-\tau)[(\rho^2-\sigma\bar{\sigma})/(\rho+\bar{\rho})]$$
$$+2\sigma(\alpha+\bar{\beta})-\sigma\bar{\tau}-\rho\tau \tag{6.19}$$

and

$$S_{12}=\begin{cases}0, & \text{for } V \text{ and } V+\Lambda,\\ 2k(\phi_1\bar{\varphi}_2+\varphi_1\bar{\phi}_2+\varphi_1\bar{\varphi}_2), & \text{for EV.}\end{cases} \tag{6.20}$$

Hence we can solve δV if

$$|(\rho^2-\sigma\bar{\sigma})^2/(\rho+\bar{\rho})|^2-\sigma\bar{\sigma}\neq 0, \tag{6.21}$$

as

$$\delta V=\omega_1 V+u_1, \tag{6.22}$$

where

$$\omega_1=\left[\left|\frac{\rho^2-\sigma\bar{\sigma}}{\rho+\bar{\rho}}\right|^2-\sigma\bar{\sigma}\right]^{-1}\left[\sigma\bar{\Omega}-\frac{\bar{\rho}^2-\sigma\bar{\sigma}}{\rho+\bar{\rho}}\Omega\right] \tag{6.23}$$

and

$$u_1=\left[\left|\frac{\rho^2-\sigma\bar{\sigma}}{\rho+\bar{\rho}}\right|^2-\sigma\bar{\sigma}\right]^{-1}\left[-\sigma\bar{S}_{12}+\frac{\bar{\rho}^2-\sigma\bar{\sigma}}{\rho+\bar{\rho}}S_{12}\right], \tag{6.24}$$

and, since $\rho+\bar{\rho}\neq 0$, we solve ΔV as

$$\Delta V=\omega_2 V-S_{22}, \tag{6.25}$$

where

$$\begin{aligned}\omega_2=&(\rho+\bar{\rho})^{-1}[\delta(\alpha+\bar{\beta}-\bar{\tau}+\tfrac{1}{2}\bar{\omega}_1)\\&+\bar{\delta}(\bar{\alpha}+\beta-\tau+\tfrac{1}{2}\omega_1)+\tfrac{1}{2}\omega_1(\bar{\omega}_1+3\alpha+5\bar{\beta}-2\bar{\tau})\\&+\tfrac{1}{2}\bar{\omega}_1(\omega_1+3\bar{\alpha}+5\beta-2\tau)+\psi_2+\bar{\psi}_2\\&-(\rho+\bar{\rho})(\gamma+\bar{\gamma})+\tfrac{1}{2}(\rho+\bar{\rho})^{-1}\mu(2\sigma\bar{\sigma}-3\rho^2+\bar{\rho}^2)\\&+1/2(\rho+\bar{\rho})^{-1}\bar{\mu}(2\sigma\bar{\sigma}-3\bar{\rho}^2+\rho^2)+(\alpha+\bar{\beta}-\bar{\tau})\\&\times(\bar{\alpha}+3\beta)+2\tau\bar{\tau}+(\bar{\alpha}+\beta-\tau)(\alpha+3\bar{\beta})\end{aligned} \tag{6.26}$$

and

$$S_{22}=\begin{cases}0, & \text{for } V \text{ and } V+\Lambda,\\ 2k\{\phi_2\bar{\varphi}_2+\varphi_2\phi_2+\varphi_2\bar{\varphi}_2\}, & \text{for EV.}\end{cases} \tag{6.27}$$

Also ϕ_i and $\phi_i+\varphi_i$ satisfy Maxwell equations [Eqs. (2.21a)–(2.21d)] in (M,g) and $(M,\tilde{g})$, respectively. Then V, in general, can be solved from Eqs. (6.12), (6.18), and (6.25).

We now return to the constraint equations (6.14) and (6.16) and investigate the existence of asymptotically flat solutions. We recall that the behavior of these space-times has been studied by Newman and Unti[25] and by Exton, Newman, and Penrose[26] for vacuum and electrovacuum fields, respectively. Using their results we obtain the following theorems.

Theorem 1: If both (M,g) and $(M,\tilde{g})$ are asymptotically flat vacuum space-times, then their Weyl tensors must be algebraically special. The GKS transform does not preserve algebraic generality transformations (see the next theorem for vacuum to electrovacuum transformations).

Proof: Following Newman and Unti[25] we can find a tetrad frame for which $\kappa=\pi=\epsilon=\rho=\bar{\rho}=\tau-\bar{\alpha}-\beta=0$. In this tetrad Eq. (6.14) has the form

$$\psi_0/\sigma=(\sigma\bar{\sigma}-\sigma^2)/\rho. \tag{6.28}$$

We write the relevant NP equations as

$$D\rho=\rho^2+\sigma\bar{\sigma}, \tag{6.29a}$$

$$D\sigma=2\rho\sigma+\psi_0. \tag{6.29b}$$

Then Eq. (6.28) gives

$$D\sigma/\sigma=D\rho/\rho=\rho+(\sigma\bar{\sigma}/\rho). \tag{6.30}$$

Solving this equation, we have $\sigma=a\rho$, where $Da=0$. Then (6.29a) gives

$$\rho(r)=[b-(1+a\bar{a})r]^{-1}=O(r^{-1}), \tag{6.31}$$

where $Db=0$, and $O(r^n)$ is the order of magnitude symbol. Thus

$$\sigma(r)=a[b-(1+a\bar{a})r]=O(r^{-1}), \tag{6.32}$$

$$\psi_0(r)=a(a\bar{a}-1)[b-(1+a\bar{a})r]^{-2}=O(r^{-2}), \tag{6.33}$$

$$V(r)=V_0[b-(1+a\bar{a})r]^{k_0}, \tag{6.34}$$

where $k_0=(1-a\bar{a})/(1+a\bar{a})$ and $DV_0=0$. It is an asymptotically flat space-time[25] $\rho=O(r^{-1})$, $\sigma=O(r^{-2})$, and $\psi_0=O(r^{-5})$, hence Eqs. (6.32) and (6.33), and shows clearly that (M,g) cannot be asymptotically flat, and, since ρ, σ, ψ_0 are invariant under the GKS transform $(M,\tilde{g})$ will have the same behavior.

Theorem 2: If (M,g) is vacuum or electrovacuum with l^μ a principal null direction (pnd) of the Maxwell tensor ($\phi_0=0$), and $(M,\tilde{g})$ a non-null ($\phi_1\neq 0$) electrovacuum space-time, their Weyl tensors are algebraically special.

Proof: Asymptotic behavior of electrovacuum space-times are given in the same tetrad frame as in the previous theorem. Then using Eqs. (6.15) and (6.29b) we have

$$\frac{D\sigma}{\sigma}=\frac{D(\psi_0/\sigma+2\rho)}{\psi_0/\sigma+2\rho}=\frac{\psi_0}{\sigma}+2\rho, \tag{6.35}$$

hence

$$\psi_0/\sigma+2\rho=(b'-r)^{-1},\quad Db'=0, \tag{6.36a}$$

$$\sigma=a'(b'-r)^{-1},\quad Da'=0, \tag{6.36b}$$

but for asymptotically flat space-times,[26] $\sigma=O(r^{-2})$, also $\rho=O(r^{-1})$ and $\psi_0=O(r^{-5})$. Therefore Eqs. (6.36a) and (6.36b) cannot be satisfied unless $\sigma=0$, i.e., (M,g) hence $(M,\tilde{g})$ are algebraically special.

VII. CONCLUSION

We expressed Einstein's equations for vacuum, vacuum with cosmological constant, and electrovacuum fields as a differential ideal using a compact Newman–Penrose formalism, and we gave two prolongations of this ideal generalizing previous works[17] to vacuum with cosmological constant and electrovacuum fields. We obtained prolongations of these ideals and constructed Bäcklund transformations. Vacuum and vacuum with cosmological constant cases were also discussed in Ref. 19.

We also gave a method to obtain Bäcklund transformations. The generalized Kerr–Schild transformation is a well-known example to these transformations. Existence of other Bäcklund transformations will also be studied.

The transformations of Newman–Penrose quantities were given in Ref. 24. We present here the (linear) differential equations for the transformation parameter for each case discussed above and show that algebraically general asymptotically flat vacuum and electrovacuum solutions cannot be obtained (starting from a vacuum solution).

We finally remark that when the space-time admits two Killing vectors, it is known that Einstein's equations constitute a completely integrable system. For space-times without symmetry, the Rarita–Schwinger equation[16,18] was proposed as an associated linear equation for Einstein's equations, therefore in the case of two Killing vectors this equation should reduce to the Belinski–Zakharov system. This problem is currently studied.

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Statistical mechanics approach in minimizing a multivariable function

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The method of minimization of a multivariable function based on the statistical mechanics analogy with a fictitious physical system of many particles is proposed. The function is assumed to be the Hamiltonian of the fictitious physical system to fit the global minimum of the function and the ground state "energy" of the fictitious system. In this model the global minimum search can be imitated by various relaxation processes in the fictitious system described by statistical mechanics. These relaxation processes lead to the equilibrium state, which is the ground state at the zero temperature limit. The imitation of a relaxation process confers to the minimization procedure the advantage of a relaxation process in a real physical system: because of thermal fluctuations a real system cannot be trapped by metastable states related to local minima. It always reaches the equilibrium state. The simulations of the relaxation processes based on the macroscopic kinetic equations and on the Monte Carlo algorithms are discussed. The new Monte Carlo algorithm based on the simulation of random walks of the representative point of the system in multidimensional phase space of the variables of the function under investigation is proposed. Unlike the conventional Metropolis–Rosenbluths–Tellers Monte Carlo method, each elementary transition in the proposed algorithm results in simultaneous movement of all atoms of the system, i.e., it generates a fluctuation involving any number of atoms.

I. INTRODUCTION

Finding the global minimum of a multivariable function is one of the most fundamental problems arising in various, often distant fields. The solution of this problem faces serious difficulties drastically increasing with number of variables. Up to now there has been no general algorithm applicable to any function. The main difficulty is that during the minimization procedure the system gets trapped in local minima. The existing minimization methods are, in fact, procedures enabling the system to escape from these traps. To our knowledge, none of these methods, however, can provide satisfactory general solution of the problem.

It should be mentioned that one example of successful solution of the minimization problem, when minimization occurs automatically and local minima do not hinder the minimization process, is given by nature. It is the case of a classical system of many particles whose potential energy, being the function of an enormous number of variables, coordinates of particles, is minimized at 0°K. The potential energy as well as most of multivariable functions has many local minima (metastable states). Nevertheless at finite temperature the system does not get trapped in the minima since thermal fluctuations enable the system to overcome potential barriers surrounding them. Therefore the system can always escape from traps and ultimately attain the global minimum if its temperature is gradually lowered.

If temperature is maintained at the same level, the system attains the global minimum of the Helmholtz free energy corresponding to the equilibrium state rather than that of potential energy. Use of the free energy at finite temperature is, in fact, equivalent to employing the "smoothing" procedure because the entropy contribution into the free energy eliminates shallow local minima of the potential energy.

The mechanisms enabling statistical mechanics systems to attain spontaneously the global minimum of the potential energy with temperature lowering are discussed here because they also can be adopted to develop the minimization procedure for an arbitrary multivariable function as efficient as that for statistical mechanics systems. For example, we may imitate a certain relaxation process in a specifically constructed model of a fictitious multiparticle physical system at finite temperature, which would lead us to the global minimum of the relevant multivariable function.

The statistical mechanics approach to the minimization of a multivariable function based on this idea was first formulated and tested in our works[1–3] for the particular problem of crystal structure determination. In this problem a multivariable function is the so-called R factor, the mean squared deviation of the calculated moduli of the structure amplitudes of x-ray diffraction reflections (Fourier transforms of scattering atomic densities) from the measured ones. The R factor is, by definition, a function of coordinates of atoms in a unit cell of the crystal lattice.

II. STATISTICAL MECHANICS FORMULATION OF THE MINIMIZATION PROCESS

Let us consider a multivariable function $E = E(x_1,x_2,...,x_N)$ of variables $x_1,x_2,...,x_N$, whose global minimum is searched. The consideration will be based on the statistical mechanics analysis of a certain fictitious multiatom system whose ground state would correspond to the global minimum of the relevant function $E(x_1,x_2,...,x_N)$. To do this, we assume that the function $E(x_1,x_2,...x_N)$ is the Hamiltonian $\hat{H}$,

$$\hat{H} = E(x_1,...,x_N), \tag{1}$$

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and the variables $x_1,...,x_N$ are coordinates of N "atoms" of a bounded fictitious one-dimensional system. This is enough to introduce the basic thermodynamic functions, the partition function Z, Helmholtz free energy Φ, and the entropy S:

$$Z = \int d\Gamma \exp\left(\frac{-E(x_1,...,x_N)}{T}\right), \tag{2}$$

where $d\Gamma = dx_1...dx_N$ is an element of phase space and T is the absolute "temperature." Integration in (2) is carried out over the bounded ranges where the variables $x_1,x_2,...,x_N$ are defined:

$$\Phi = -T\ln Z, \tag{3}$$

$$S = \ln \Gamma(\overline{E}), \tag{4}$$

where

$$\overline{E} = \langle E \rangle_\infty = \int d\Gamma \frac{1}{Z} \exp\left(\frac{-E(x_1,...,x_N)}{T}\right) E(x_1,...,x_N)$$

is the internal energy, $\langle \cdots \rangle_\infty$ denotes averaging over a thermodynamic ensemble, and $\Gamma(\overline{E})$ is the "area" of the hypersurface

$$E(x_1,...,x_N) = \overline{E}.$$

The free energy (3) also can be represented in another form:

$$\Phi = \overline{E} - TS. \tag{5}$$

The temperature T introduced in (2)–(5) characterizes the degree of "excitation" of the system. All the introduced thermodynamic functions are related to the equilibrium state. To describe both equilibrium and nonequilibrium states it is convenient to introduce correlation functions of the system.

If the system finds itself in the equilibrium state, one-particle correlation functions, "atomic densities" $\rho_i(x_i,\infty)$, $i = 1,2,...,N$, are described by the equation

$$\rho_i(x_i,\infty) = \int dx_1 \cdots dx_{i-1}\, dx_{i+1} \cdots dx_N \times \frac{1}{Z} \exp\left(\frac{-E(x_1,...,x_N)}{T}\right),$$

following from the Gibbs distribution. If the system has not reached the equilibrium state yet, its atomic distribution is described by nonequilibrium densities $\rho_i(x_i)$, which can be found by solution of the kinetic equations for correlation functions. The densities $\rho_i(x_i)$, by definition, meet the normalization conditions

$$\int \rho_i(x_i)dx_i = 1. \tag{6}$$

The internal energy of both equilibrium and nonequilibrium states can be expressed through the N-particle correlation function $\rho(x_1,...,x_N)$ as follows:

$$E = \langle E \rangle = \int dx_1 \cdots dx_N\, \rho(x_1,...,x_N)E(x_1,...,x_N), \tag{7}$$

where $\langle \cdots \rangle$ denotes the averaging procedure. For the equilibrium state the N-particle correlation function $\rho(x_1,...,x_N;\infty)$ is given by the Gibbs distribution itself:

$$\rho(x_1,...,x_N,\infty) = (1/Z)\exp(-E(x_1,...,x_N)/T). \tag{8}$$

Nonequilibrium entropy in terms of correlation function has the form

$$S = -\int dx_1 ... dx_N\, \rho(x_1,...,x_N)\ln\rho(x_1,...,x_N). \tag{9}$$

All calculations are strongly simplified in the mean field approximation. Transition to the mean field approximation is carried out by means of decoupling,

$$\rho(x_1,x_2,...,x_N) \simeq \rho_1(x_1)\rho_2(x_2)\cdots\rho_N(x_N), \tag{10}$$

which implies neglecting fluctuations in the system. Approximation (10) is asymptotically correct at the extreme case of low temperatures, which is the case of interest.

With the mean field approximation (10) the internal energy (7) has the form

$$\overline{E} \simeq \int dx_1 \cdots dx_N\, \rho_1(x_1)\cdots\rho_N(x_N)E(x_1,...,x_N). \tag{11}$$

The entropy (8) is transformed into

$$S \simeq -\sum_{i=1}^{N} \int \rho_i(x_i)\ln\rho_i(x_i)dx_i \tag{12}$$

if normalization conditions (6) are taken into account. Making use of (11) and (12) in (5), one obtains the equation for the free energy:

$$\Phi = \overline{E} - TS = \int d\Gamma\, E(x_1,...,x_N)\rho_1(x_1)\cdots\rho_N(x_N) + T\sum_{i=1}^{N}\int \rho_i(x_i)\ln\rho_i(x_i)dx_i. \tag{13}$$

Equilibrium densities, $\rho_i(x_i)$ are known to be determined by the global minimum of the free energy Φ. The necessary minimum condition for the free energy under the conservation conditions (6) yields the set of N nonlinear integral equations:

$$\frac{\delta}{\delta\rho_i(x_i)}\left[\Phi - \sum_{j=1}^{N}\mu_j\int\rho_j(x_j)dx_j\right] = \frac{\delta\Phi}{\delta\rho_i(x_i)} - \mu_i = 0, \tag{14}$$

where, according to (11) and (12),

$$\frac{\delta\Phi}{\delta\rho_i(x_i)} = \frac{\delta\overline{E}}{\delta\rho_i(x_i)} + T\ln\rho_i(x_i) = T\ln\rho_i(x_i) + \int' dx_1\cdots dx_{i-1}\, dx_{i+1}\cdots dx_N \times E(x_1,...,x_N)\rho_1(x_1)\cdots\rho_{i-1}(x_{i-1}) \times\rho_{i+1}(x_{i+1})\cdots\rho_N(x_N), \tag{15}$$

and μ_i is the undetermined Lagrange multiplier (chemical potential) of the ith atom. The chemical potentials μ_i should be, as usual, chosen to provide the conservation conditions (6). As was mentioned above, the equilibrium free energy, $\Phi_{\min}$, tends to $E_{\min}$ ($\Phi_{\min}\to E_{\min}$) with $T\to 0$, where $\Phi_{\min}$ and $E_{\min}$ are global minima of the free energy and potential energy, respectively. Therefore minimization of the free energy (12) with respect to the densities $\rho_1(x_1),\rho_2(x_2),...,\rho_N(x_N)$ at gradually lowering temperature solves the problem of minimization of the function $E(x_1,...,x_N)$ with respect to the variables $x_1,...,x_N$. In other words, the statistical mechanics approach formulated above enables us to substi-

tute minimization of the function $E(x_1,...,x_N)$ with respect to its variables $x_1,x_2,...,x_N$, for minimization of the functional Φ with respect to N densities, $\rho_1(x_1),...,\rho_N(x_N)$.

The question of whether such a substitution improves our chances to obtain the global minima will be discussed below.

It is of interest also to notice that the above-formulated minimization method dealing with the free energy of the system is equivalent to the application of the maximum entropy principle. Indeed, maximizing the entropy S under the condition that the function $\bar{E}$ should be minimal amounts to minimizing the function

$$\varphi = -S + \lambda \bar{E}, \tag{16}$$

where λ is the undetermined Lagrange multiplier. If the Lagrange multiplier $\lambda = 1/T$ is introduced, Eq. (16), in fact, becomes equivalent to the equation $\Phi = \bar{E} - TS$ for the free energy utilized above.

III. MINIMIZATION BY MEANS OF IMITATION OF MACROSCOPIC RELAXATION

The statistical mechanics analogy proposed above for solution of the mathematical problem of minimizing a function of multiple variables may be extended not only to thermodynamics but also to kinetics. In the latter case, a spontaneous relaxation process for density functions, $\rho_1(x_1),...,\rho_N(x_N)$, resulting in a decrease in free energy (13) and consequently leading to the equilibrium state referred to the global minimum of the free energy, can be simulated. In many cases this approach seems to be more efficient than the direct numerical solution of the set of nonlinear equations (14). The relaxation process can be, for example, described by the Önsager equations, which, after neglecting the off-diagonal kinetic coefficients, have the following form:

$$\frac{d\rho_i(x_i,t)}{dt} = -L\left[\frac{\delta\Phi}{\delta\rho_i(x_i)} - \mu_i\right], \tag{17}$$

where L is the diagonal Önsager coefficient, $\delta\Phi/\delta\rho_i(x_i) - \mu_i$ is the thermodynamic driving force, and t is "time." It is noteworthy that (17) is, in fact, the basic equation of the gradient method. Using (15) in (17) and choosing a "time" scale so that L is equal to unity, we have

$$\begin{aligned}\frac{d\rho_i(x_i,t)}{dt} &= -\Big[T\ln\rho_i(x_i) - \mu_i \\ &\quad + \int' dx_1 \cdots dx_{i-1}\, dx_{i+1} \cdots dx_N E(x_1,...,x_N) \\ &\quad \times \rho_1(x_1)\cdots\rho_{i-1}(x_{i-1})\rho_{i+1}(x_{i+1})\cdots\rho_N(x_N)\Big], \\ &\quad \text{at } i = 1,...,N.\end{aligned} \tag{18a}$$

Since (18a) describes the system with a variable number of atoms, it is convenient to supplement it with an equation for chemical potentials:

$$\frac{d\mu_i}{dt} = -\frac{1}{\tau}\left[\int \rho_i(x_i,t)dx_i - 1\right], \quad \text{at} \quad i = 1,...,N, \tag{18b}$$

providing fulfillment of the normalization conditions (6) in the sought equilibrium state. The relaxation "time" τ should be chosen to be comeasureable with the typical relaxation time of the entire system.

Equation (18) in such a general form can be of practical use only if the number of integrations in its right-hand side does not exceed 1. It is certainly not the case with a general function $E(x_1,...,x_N)$. Let us formulate the specific cases when the kinetic equations can be solved numerically without computation of multiple integrals. The number of integrations in (18) does not exceed unity if the function E is a sum of pairwise functions $W_{ij}(x_i,x_j)$:

$$E(x_1,...,x_N) = \sum_{i>j=1}^{N} W_{ij}(x_i,x_j). \tag{19}$$

In this case Eq. (18a) is simplified to

$$\begin{aligned}\frac{d\rho_i(x_i,t)}{dt} = -\Big[&\sum_{j=1}^{N}\int W_{ij}(x_i,x_j)\rho_j(x_j)dx_j \\ &+ T\ln\rho_i(x_i) - \mu_i\Big].\end{aligned} \tag{20}$$

Kinetic equations can also be solved in another specific case when

$$E(x_1,...,x_N) = \Psi\Big(\sum_{i=1}^{N}\varphi_i(x_i)\Big), \tag{21}$$

where $\Psi(X)$ and $\varphi_i(x)$ are quite general functions. In the case (21) the mean field approximation yields

$$\begin{aligned}\bar{E} &= \Big\langle\Psi\Big(\sum_{i=1}^{N}\varphi_i(x_i)\Big)\Big\rangle \approx \Psi\Big(\sum_{i=1}^{N}\langle\varphi_i(x_i)\rangle\Big) \\ &= \Psi\Big(\sum_{i=1}^{N}\int\varphi_i(x_i)\rho_i(x_i)dx_i\Big).\end{aligned} \tag{22}$$

Since Eq. (18a) can be presented as

$$\frac{d\rho_i(x_i,t)}{dt} = -\left[\frac{\delta\bar{E}}{\delta\rho_i(x_i)} + T\ln\rho_i(x_i) - \mu_i\right], \tag{23}$$

we may rewrite (23) as

$$\begin{aligned}\frac{d\rho_i(x_i,t)}{dt} = -\Big[&\Psi'\Big(\sum_{i=1}^{N}\int\varphi_i(x_i)\rho_i(x_i)dx_i\Big)\varphi_i(x_i) \\ &+ T\ln\rho_i(x_i,t) - \mu_i\Big],\end{aligned} \tag{24}$$

if the mean field approximation (22) is employed in (23).

Equation (24) includes the sole integration on its right-hand side and thus, in principle, can be solved numerically.

The particular case similar to that given by (24) was considered previously in our above-cited papers,[1,2] where the thermodynamic concept for the minimization procedure was first proposed. It is related to the crystal structure determination problem based on the minimization of the R factor, a multivariable function of atomic coordinates in a unit cell of the crystal lattice. In this case

$$E = R(\mathbf{r}_1,\cdots\mathbf{r}_N) = \sum_{\mathbf{H}}(|F(\mathbf{H};\mathbf{r}_1,...,\mathbf{r}_N)|^2 - I(\mathbf{H}))^2, \tag{25}$$

where

$$F(\mathbf{H};\mathbf{r}_1,...,\mathbf{r}_N) = \sum_{j=1}^{N} \varphi_j(\mathbf{H},\mathbf{r}_j), \tag{26}$$

$$\varphi_j(\mathbf{H},\mathbf{r}_j) = f_j \exp(i2\pi\mathbf{H}r_j) \quad \text{[compare with (21)]},$$

where the $\mathbf{r}_j = (x_j,y_j,z_j)$ are coordinates of the jth atom in the unit cell and f_j, $I(\mathbf{H})$, and $\mathbf{H}$ are known constants: the atomic scattering factor of the jth atom and the observed intensity $I(\mathbf{H})$ of the diffraction reflection related to the reciprocal lattice vector $\mathbf{H}$. In the case (25) Eq. (22) has the form

$$\overline{E} = \sum_{\mathbf{H}} \left[\left| \sum_{j=1}^{N} f_j \langle \exp(i2\pi\mathbf{H}\mathbf{r}_j) \rangle \right|^2 - I(\mathbf{H}) \right]^2$$

$$= \sum_{\mathbf{H}} \left[\left| \sum_{j=1}^{N} f_j \int \rho_j(r_j) \exp(i2\pi\mathbf{H}\mathbf{r}_j) d^3\mathbf{r}_j \right|^2 - I(\mathbf{H}) \right]^2. \tag{27}$$

Solution of the same problem of crystal structure determination based on another idea, the maximum entropy principle, was later proposed in several works.[4–7] But, as a matter of fact, there is no difference between the maximum entropy approach and thermodynamic approach proposed earlier. The apparent difference consists in terminology only, because, as was shown by Navazo, Castellano, and Tsoucaris,[8] employing the entropy maximization instead of the free energy minimization results in the same optimization equations (see also the end of Sec. I).

Summing up the foregoing results, one can see that the thermodynamic approach based on the imitation of the macroscopic relaxation of the system of many particles is valid for minimization of very specific multivariable functions: In the general case each iteration of numerical calculations would require multiple integrating, the procedure being too formidable to be successfully carried out. The second difficulty is even more fundamental. Minimizing the free energy at a finite temperature rather than the "Hamiltonian" $E(x_1,...,x_N)$ may remove shallow local minima as was mentioned before, but there is no guarantee that it removes all local minima at all. In the latter case the system may be trapped in a remaining deep local minimum and fail to reach the global one.

The method proposed in the next section seems to be free from the shortcomings mentioned above. This method is based on the Monte Carlo simulation of microscopic processes of atomic migrations driving the system to its equilibrium state. It can be successfully used even for the function $E(x_1,...,x_N)$ taken in a general form.

The simulation of thermal fluctuations inherent to a Monte Carlo scheme enables the system to escape local minima and ultimately attain the global minimum.

IV. MINIMIZATION BY MEANS OF MONTE CARLO SIMULATION OF RELAXATION PROCESS

Let us consider the microscopic relaxation process leading to the equilibrium state corresponding to the free energy minimum, which is simulated by the Monte Carlo method. Finding the equilibrium state at a low temperature would also solve the minimization problem since the most probable microstates of a system at low temperature are known to be close to the ground state, the global minimum of the "Hamiltonian" $E(x_1,...,x_N)$. The Monte Carlo sampling scheme similar to that proposed first by Metropolis, the Rosenbluths, and the Tellers for a gas of interacting atoms[9] (the MRT method) and later widely used for many statistical mechanics applications[10] serves this purpose.

Let us assume that coordinates of N "atoms," $x_1,x_2,...,x_N$, are coordinates of the representative point of a relevant fictitious atomic system in N-dimensional phase space. The proposed Monte Carlo method consists of simulation of random walks of the representative point within phase space rather than one-by-one random walks of atoms in real space as in the MRT method. Random walks are generated by means of constant stepwise probabilities for elementary transitions that produce a succession of points in phase space enumerated by number t. These transitions form a Markov chain. Probabilities of elementary atomic transitions are chosen so that any mean value taken over a segment of the Markov chain that starts from a certain point of phase space, remote from the beginning of the chain, would tend to the mean value taken over the petite canonical ensemble with the given model Hamiltonian $E(x_1,...,x_N)$ if the segment length tends to infinity.

Below the brief account of the proposed Monte Carlo algorithm generating such a chain is presented.

Let the representative point occupy a point $\mathbf{R}(t) = (x_1,x_2,...,x_N)$ at the "time" t. The next point, $\mathbf{R}'(t+1) = (x_1',x_2',...,x_N')$, in which the representative point is shifted to form the $(t+1)$th state, is generated as follows.

(1) N random numbers $(\xi_1,\xi_2,...,\xi_N)$ are generated so that each of them is uniformly distributed within the interval $[0,1]$.

It gives us the shift vector $\mathbf{h} = a(\xi_1,\xi_2,...,\xi_N)$ randomly distributed within the N-dimensional hypercube of edge length a, which produces the elementary transition $\mathbf{R}(t) \rightarrow R'(t+1)$ according to equation

$$\mathbf{R}'(t+1) = \mathbf{R}(t) + \mathbf{h},$$

i.e.,

$$R'(t+1) = (x_1,x_2,...,x_N) + a(\xi_1,\xi_2,...,\xi_N)$$

$$= (x_1 + a\xi_1, x_2 + a\xi_2,...,x_N + a\xi_N). \tag{28}$$

Therefore the random number generator enables us to select a new point $\mathbf{R}'(t+1)$ in which the representative point may be shifted from the point $\mathbf{R}(t)$ during the elementary transition.

To answer whether or not the representative points shifts by $\mathbf{h}$ from the point $\mathbf{R}(t)$ to the selected new point $\mathbf{R}'(t+1)$, the next step should be done.

(2) The change in "energy"

$$\Delta E = E(x_1 + a\xi_1, x_2 + a\xi_2,...,x_N + a\xi_N) - E(x_1,...,x_N)$$

resulting from the elementary transition

$$(x_1,x_2,...,x_N) \rightarrow (x_1 + a\xi_1, x_2 + a\xi_2,...,x_N + a\xi_N)$$

of the representative point is computed. Two outcomes are then possible.

(i) If $\Delta E \leqslant 0$, the elementary transition is made and the resultant atomic configuration corresponding to the representative point

$$\mathbf{R}'(t+1) = (x_1 + a\xi_1, x_2 + a_2\xi_2, \ldots, x_N + a\xi_N)$$

is assumed to be the new one.

(ii) If $\Delta E > 0$, the elementary transition $\mathbf{R}(t) \to \mathbf{R}'(t+1)$ is made with the probability $\exp(-\Delta E/T)$. It occurs if a number ξ taken from a uniform distribution on the interval [0,1] produced by the random number generator satisfies the inequality $\xi < \exp(-\Delta E/T)$, and it does not occur if $\xi \geqslant \exp(-\Delta E/T)$. In both cases the resultant configuration is assumed to be the new one.

It can be easily proved that the proposed Monte Carlo scheme generates a Markov chain of microstates $\mathbf{R}(t)$. The mean value of any physical value $A = A(x_1(t), \ldots, x_N(t)) = A(\mathbf{R}(t))$ over the stationary segment of the Markov chain between the t_0th and $(t_0 + t)$th states tends to its mean value over the petite canonical ensemble when $t \to \infty$, i.e.,

$$\frac{1}{t}\sum_{\tau=t_0}^{t_0+t} A(\mathbf{R}(\tau)) \to \int dx_1 \ldots dx_N \, A(\mathbf{R}) \frac{1}{Z} \exp\left(-\frac{E(\mathbf{R})}{T}\right). \tag{29}$$

The proof of relation (29) is the same as that for the MRT method (see, for example, the review paper by Wood[11]). The main difference, which, however, does not change the line of reasoning, is that in the relevant case we consider migration of the representative point in N-dimensional phase space, whereas in the case of the MRT method, migration of atoms occurs one by one.[12] In both cases the assumption that atomic coordinate variations are bounded is needed, however. It should also be mentioned that the MRT scheme is a particular case of the scheme formulated above. Indeed, the former can be obtained from the latter by imposing the quite rigid constraint on elementary transitions, viz. the assumption that each elementary transition of a representative point can occur only along one of N coordinate axes of the N-dimensional phase space of the system. Only such a constraint yields an elementary transition involving a sole atom as it is required by the MRT algorithm. On the contrary, each elementary transition generated in the method proposed above involves simultaneous migration of all atoms and thus has a more general form. In terms of fluctuations this difference can be formulated as follows. The MRT method generates fluctuations resulting in the movement of a sole atom and does not take into account fluctuations of pairs, triplets, quadruplets, and so on of atoms, whereas a fluctuation generated by the relevant method are more general: it may involve any number of atoms. Because of this, the better convergence of the relevant Monte Carlo algorithm should be expected. If it is true, the proposed algorithm wil prove to be more efficient also for conventional statistical mechanics systems than that of the MRT method usually employed. The results already obtained are quite promising. The thermodynamics analogy proposed in Refs. 1 and 2 was the basis for the structure determination of a crystal from the x-ray diffraction data[3] and for solution of the traveling salesman problem.[13] In both cases the MRT method was applied for a certain fictitious multiatom physical system. Minimization of a multivariable function in both studies would be impossible to obtain by conventional mathematic methods. Employing the relevant Monte Carlo technique seems to be even more promising.

For a very important problem, crystal structure determination from x-ray diffraction data, the Monte Carlo approach based on the thermodynamic analogy raises the hope of a breakthrough in the problem of direct determination of a structure of a crystal with more than 100 atoms per unit cell and the even more ambitious problem of protein structure determination without heavy atom derivatives. In the latter case the relevant Monte Carlo method may be applied successively in several stages, increasing the resolution from stage to stage.

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R-mer filling with general range-*R* cooperative effects

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An exact closed form solution is obtained for the time dependence of the coverage of a homogeneous, infinite, one-dimensional lattice filled irreversibly and cooperatively by R-mers. Cooperative effects, *not* assumed to be reflection invariant, may extend up to range R. Previously available exact solutions for random filling and nearest neighbor cooperative effects are recovered. For dimer filling with genuine range-2 cooperative effects it is found that autoretardative and autocatalytic rate regimes may lead to the *same* saturation coverage. Various adsorption schemes are considered.

I. INTRODUCTION

As indicated recently,[1] the problem of R-mer filling with general range-R cooperative effects is exactly solvable. A method of solution[1-6] deals with an infinite hierarchy of rate equations for the various subconfiguration probabilities, reduces it to a closed subhierarchy for $f_n(t)$, $n = 1,2,...$, the average densities of sequences of n contiguous empty sites at time t, and achieves exact hierarchy truncation[1-3] on observing an empty site shielding property.[1,2] In the present case, a closed coupled set of hierarchical equations for $f_1(t),...,f_{3R-1}(t)$ is retained. This system of $3R-1$ first-order linear differential equations can be integrated recursively, but it is not clear[1] whether successive solution is suited for providing closed form expressions for $f_n(t)$, $n = 1,...,3R-1$.

The lattice coverage[1-6] at time t, $\theta(t)$, is of great importance both in the study of adsorption processes[7] as well as in the analysis of reactions on polymer chains,[8] and it is this quantity we are interested in. It is given by the relation

$$\theta(t) = 1 - \sum_{n=1}^{\infty} n f_n(t) \tag{1}$$

and may therefore be obtained from the above-mentioned approach.[1] The fact that Eq. (1) involves an infinite sum is not really a problem since $\Sigma_{n=3R}^{\infty} n f_n(t)$ is of simple form,[1] but in making use of Eq. (1), $f_1(t),...,f_{3R-1}(t)$ clearly must be known. Rather than to explore the possibility of obtaining explicit representations for $f_1(t),...,f_{3R-1}(t)$, and hence for $\theta(t)$, we here present a generating function technique[4,5,9-13] that yields $\theta(t)$ directly. The quantity we study is the mean number $N_n(t)$ of empty sites at time t in a lattice of n initially unoccupied compartments (sites). Imposing some simplifying boundary condition (which has no effect in the limit of an infinite lattice) it is seen that $dN_n(t)/dt$ may be expressed in terms of $N_1(t),...,N_n(t)$. These first-order linear differential equations, beginning with $n = R$ [observe that trivially $N_1(t) \equiv 1,...,N_{R-1}(t) \equiv R-1$], may be integrated progressively. However, solving successively does not seem to be quite suitable to perform an asymptotic analysis. We thus introduce a generating function for $\{N_n(t)\}$, which proves to satisfy a first-order linear partial differential equation whose solution, subject to an appropriate initial condition, can be obtained explicitly, providing precise information on the asymptotic behavior $(n \to \infty)$ of $N_n(t)$ and, particularly, on

$$\theta(t) = 1 - \lim_{n\to\infty} N_n(t)/n. \tag{2}$$

Exact closed form solutions for irreversible cooperative processes on infinite one-dimensional lattices have been given by several workers (see Ref. 1 for a review). In all the cases treated, the lattice coverage $\theta(t)$ [a similar remark applies to $f_n(t)$] is found to be of the generic form

$$\theta(t) = \Phi^*(t) + \sum_{i=1}^{\kappa} \Phi_i(t) \int_{e^{-\lambda t}}^{1} P_i(x) x^{b_i} e^{Q(x)}\, dx, \tag{3}$$

where P_i and Q are polynomials, Φ^* and Φ_i are (possibly constant) functions of exponential type, and $\lambda > 0$, κ, and b_i are constants. As we shall see in Sec. V, processes with general range-R cooperative effects will, for the most part, obey that rule as well. Only in some exceptional cases P_i may *not* be a polynomial. In the case of random R-mer filling,[9] the polynomial Q is of order $R-1$; it is of order R for R-mer filling with nearest neighbor cooperative effects[4] as well as in the case of the isomorphic[1] process of monomer filling with range-R cooperative effects incorporating range-$(R-1)$ blocking.[5] We shall find in Sec. V that for R-mer filling with genuine range-R cooperative effects the order of Q raises to $2R-1$. Thus, with the exception of Flory's random dimer filling[14,15] and Boucher's monomer filling with nearest neighbor cooperative effects,[16] the integral on the right-hand side (rhs) of Eq. (3) must be evaluated numerically.

By simply performing an integration by parts in Eq. (3) it is seen that Φ^*, Φ_i, P_i, and b_i are *not* uniquely determined. Their actual form, however, may be of considerable importance. For example, $b_i < 0$ may cause convergence problems[4] of numerical quadrature procedures; even worse, $b_i \leqslant -1$ may (additionally) complicate an asymptotic $(t \to \infty)$ analysis; for integration purposes, however, a high-order polynomial P_i is not desirable either. In consequence, it is worthwhile to know that the present approach is highly ambiguous in the sense that it may produce quite a lot of different integral representations (3). This peculiarity[10,11] of the generating function technique (see Appendix A) is due to the following. Since the divergence behavior of $F_k(s,t) = \Sigma_{n=k}^{\infty} N_n(t) s^n$ as $s \uparrow 1$ [which determines the

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asymptotic behavior of $N_n(t)$ as $n\to\infty$] does obviously not depend on $k = 1,2,...$, *any* F_k may be chosen as "the" generating function. But to each F_k $(k = R, R+1,...)$ corresponds an integral representation (3) with characteristic Φ^*, Φ_i, P_i, and b_i (i.e., these quantities depend on k). In Sec. IV, two possible choices

$$G_1(s,t) = \sum_{n=3R}^{\infty} N_n(t)s^n \tag{4}$$

and

$$G_2(s,t) = \sum_{n=R}^{\infty} N_n(t)s^n \tag{5}$$

will be dealt with. The integral representation (3) associated with G_1 is of "all-weather" type ($b_i > 0$), well suited for inhibitory like effects, but unnecessarily monstruous (high-order P_i) for autocatalytic processes and random filling. The generating function G_2 leads to an integral representation (3), which converges badly if effects are anticooperative. It is, however, well adapted for autocatalytic rates and reduces to a well-known representation[10,11] in the case of random filling. A further possibility (not explored here) is to consider $M_n(t) = n - N_n(t)$ (the average number of *occupied* sites at time t in a lattice of n initially empty compartments) and some corresponding generating function. Tackling the problem this way also affects[10,11] the representation (3), though *not* altering its generic form.

R-mer filling with general range-R^* cooperative effects, $R^* > R$, is *not* amenable to exact solution.[1-3,17] As a consequence, our method *cannot* go through in this case either. That this is indeed so will be seen in Appendix B.

In the following section (Sec. II) we introduce some notation and define the model precisely. The rate equations for $N_n(t)$ are stated in Sec. III and transformed into partial differential equations for the generating functions G_1 and G_2 in Sec. IV. Closed form expressions for $\theta(t)$ are given in Sec. V. Various examples of cooperative processes are discussed in Sec. VI.

II. THE MODEL

Given a linear lattice of sites, which may be either filled or empty, we call a run of k adjacent *empty* sites a *k-tuplet* and term a maximal k-tuplet (i.e., a k-tuplet not forming part of any larger n-tuplet, $n \geqslant k+1$) a *k-gap*. Observe that a k-tuplet contains k singlets, $k-1$ doublets,..., and two $(k-1)$-tuplets.

Since the present R-mer filling process is assumed to be irreversible and since multiple occupation of sites will not be considered, the state of the lattice can change only by adsorption of R-mers to R-tuplets, i.e., by occupying R contiguous *empty* sites at a time. Adsorption rates, thus clearly referring to R-tuplets, will generally be influenced by the occupied or unoccupied status of other sites on the lattice. In this paper we shall assume that these cooperative effects are restricted to range R, i.e., the $(R+1)$st, $(R+2)$nd,... nearest neighbors on either side of an R-tuplet do not affect its adsorption rate.

Because of R-mer filling, if an R-tuplet's $(k \leqslant R-1)$ nearest neighbor is occupied, its $(k+1)st,...,R$ th nearest neighbors (on the same side) are filled, too. The *range-R environment* of an R-tuplet is therefore completely described by a pair (i,j) of non-negative integers, $i,j \leqslant R$, denoting by i and j the number of *empty* neighboring sites (within range R) to the left and right, respectively. Since there are $(R+1)^2$ possible range-R environments we must specify an equal number of adsorption rates to completely characterize the process. The adsorption rates associated with the range-R environment (i,j) will be denoted $\tau_{i,j}$ and assumed to be time independent. We furthermore assume that $\tau_{R,R} > 0$.

The present generating function technique requires the study of *finite* lattices. Then, in contrast to infinite lattices, end effect problems[18] come up. These, however, are overcome most easily by considering only lattices with R filled units at each end.[4,5] Such a boundary condition (as any other referring to a finite number of end sites) has no effect on an asymptotic $(n\to\infty)$ analysis.

We are now in a position to define our adsorption process formally. Fix an integer $R \geqslant 1$ and consider a homogeneous one-dimensional lattice of $n+2R$ sites. Suppose that the R contiguous units at both its ends are occupied while its remaining n interior sites are initially $(t=0)$ empty. Regarding the kinetics of the filling process we then postulate that an R-tuplet with range-R environment (i,j),present at time $t \geqslant 0$, becomes occupied in the time interval $(t, t+h)$ with probability $\tau_{i,j}h + o(h)$ [as usual, $o(h)$ stands for a quantity of smaller order of magnitude than h, i.e., $o(h)$ is such that $o(h)/h \to 0$ as $h \to 0$], and there is no desorption from the lattice, no multiple occupation of sites, and no skating across the lattice. The time development of the lattice coverage will be described by $N_n(t)$, the average number of empty sites at time t. Clearly,

$$N_n(0) = n, \quad n = 0,1,..., \tag{6}$$

$$N_n(t) \equiv n, \quad n = 0,1,...,R-1, \quad t \geqslant 0. \tag{7}$$

It is convenient to introduce the following notations:

$$\tau = \tau_{R,R} > 0 \tag{8}$$

$$\tau_j = \tau_{R,j} + \tau_{j,R}, \quad j = 0,1,...,R-1, \tag{9}$$

$$\tau_{i,j} = \begin{cases} \tau, & \text{if } i,j \geqslant R, \\ \tau_{i,R}, & \text{if } j \geqslant R \text{ and } i = 0,1,...,R-1, \\ \tau_{R,j}, & \text{if } i \geqslant R \text{ and } j = 0,1,...,R-1, \end{cases} \tag{10}$$

$$d_k = \sum_{i=0}^{k} \tau_{k-i,i}, \quad k = 0,1,..., \tag{11}$$

$$\rho = \sum_{i=0}^{R-1} \frac{\tau_i}{\tau} \quad \text{and} \quad \gamma = 3R - 1 - \rho. \tag{12}$$

In our filling process, the adsorption of an R-mer may be viewed as the destruction of some k-gap, say, and the simultaneous creation of a (left-hand) k_1-gap and a (right-hand) k_2-gap, $k_1 + k_2 + R = k$. Observe that the destruction of a $(k+R)$-gap takes place at rate d_k.

For later reference we state

$$\sum_{i=1}^{k} i(\tau_{i,k-i} + \tau_{k-i,i}) = kd_k, \quad k = 1,2,..., \tag{13}$$

$$\sum_{i=0}^{R-1} \tau_i = d_{2R-1} = \tau\rho. \tag{14}$$

To prove Eq. (14) we rewrite d_{2R-1} [see Eq. (11)] in the form

$$d_{2R-1}=\sum_{i=0}^{R-1}\tau_{2R-1-i,i}+\sum_{i=R}^{2R-1}\tau_{2R-1-i,i}$$

and observe that

$$\sum_{i=R}^{2R-1}\tau_{2R-1-i,i}=\sum_{i=0}^{R-1}\tau_{R-i-1,i+R}=\sum_{i=0}^{R-1}\tau_{R-i-1,R}=\sum_{i=0}^{R-1}\tau_{i,R}$$

and

$$\sum_{i=0}^{R-1}\tau_{2R-i-1,i}=\sum_{i=0}^{R-1}\tau_{R,i},$$

where we used (10) twice. On recalling (9), Eq. (14) follows.

III. THE RATE EQUATIONS

The following rate equations are fundamental to our subsequent analysis (they will be derived in Appendix B):

$$\frac{dN_n(t)}{dt}=-\left[(n-3R+1)\tau+\sum_{j=0}^{R-1}\tau_j\right]N_n(t)+2\tau\sum_{j=R}^{n-2R}N_j(t)+\sum_{j=0}^{R-1}\tau_j[j+N_{n-j-R}(t)],\quad n\geq 3R-1. \tag{15}$$

In Appendix B we will see furthermore that

$$N_{n+R}(t)=n+Re^{-d_nt},\quad n=0,1,\ldots,R-1, \tag{16}$$

and

$$N_{n+2R}(t)=q_{n+R}+(r_{n+R}+p_{n+R}t)e^{-d_{n+R}t}+\sum_{i=0}^{n}a_{n,i}e^{-d_it},\quad n=0,1,\ldots,R-1, \tag{17}$$

where we set, for any $n=0,1,\ldots,R-1$,

$$q_{n+R}=\begin{cases}n+R-\dfrac{R}{d_{n+R}}\displaystyle\sum_{i=0}^{n}\tau_i, & \text{if } d_{n+R}\neq 0,\\ 0, & \text{if } d_{n+R}=0;\end{cases} \tag{18}$$

$$a_{n,i}=\begin{cases}R\tau_{n-i}/(d_{n+R}-d_i), & \text{if } d_i\neq d_{n+R},\\ 0, & \text{if } d_i=d_{n+R},\end{cases}\quad i=0,1,\ldots,n; \tag{19}$$

$$r_{n+R}=n+2R-q_{n+R}-\sum_{i=0}^{n}a_{n,i}; \tag{20}$$

and

$$p_{n+R}=R\sum_{i\in M_n}\tau_{n-i}, \tag{21}$$

with $M_n=\{i=0,1,\ldots,n\,|\,d_i=d_{n+R}\neq 0\}$. Note that if $d_{n+R}=0$, then necessarily $\tau_i=0$, $i=0,\ldots,n$, and hence $a_{n,i}=0$ whether $d_i=d_{n+R}=0$ or not. Furthermore, p_{n+R} may differ from zero only if $d_{n+R}\neq 0$. Thus, if $d_{n+R}=0$ then $N_{n+2R}(t)=n+2R$ as it should.

By making use of (16) and (17), Eq. (15) may be integrated recursively, thus providing closed form solutions [see also Eq. (47)] for finite lattices (of the form considered here). Proceeding this way, however, does not seem to be suitable to analyze infinite lattices. We therefore employ the following generating function technique.

IV. DIFFERENTIAL EQUATIONS FOR THE GENERATING FUNCTIONS G_1 AND G_2

We first deal with G_1 as defined in Eq. (4). Multiplying both sides of Eq. (15) by s^n and summing from $3R$ to ∞ gives

$$\frac{\partial G_1}{\partial t}+\tau s\frac{\partial G_1}{\partial s}=\tau\left[\gamma+\frac{s^Rg_0(s)}{1-s}\right]G_1+R_1(s,t), \tag{22}$$

where γ has been introduced in Eq. (12) and where

$$g_0(s)=(1/\tau)\{\tau_0+(\tau_1-\tau_0)s+\cdots+(\tau_{R-1}-\tau_{R-2})s^{R-1}+(2\tau-\tau_{R-1})s^R\} \tag{23}$$

and

$$R_1(s,t)=\sum_{i=0}^{R-1}\tau_is^{R+i}\sum_{n=2R-i}^{3R-1}s^nN_n(t)+\left\{2\tau\sum_{i=R}^{3R-1}s^{i+2R}N_i(t)+s^{3R}\sum_{i=0}^{R-1}i\tau_i\right\}(1-s)^{-1}.$$

Furthermore, setting

$$g_k(s)=\begin{cases}\dfrac{1}{\tau}\left\{\tau_k+\displaystyle\sum_{i=1}^{R-k-1}(\tau_{k+i}-\tau_{k+i-1})s^i+(2\tau-\tau_{R-1})s^{R-k}\right\}, & k=1,\ldots,R-1,\\ 2, & k=R,\end{cases} \tag{24}$$

we may rewrite $R_1(s,t)$ in the form

$$R_1(s,t)=\frac{s^{3R}}{1-s}\left\{\sum_{i=1}^{R-1}i\tau_i+\tau\sum_{n=0}^{R-1}g_{R-n}(s)N_{n+R}(t)+\tau g_0(s)\sum_{n=0}^{R-1}s^nN_{n+2R}(t)\right\}. \tag{25}$$

This in turn, on substituting for $N_{n+R}(t)$ and $N_{n+2R}(t)$ from (16) and (17), respectively, may be transformed into

$$R_1(s,t)=\frac{\tau s^{3R}}{1-s}\left\{\delta_1(s)+\sum_{i=0}^{2R-1}\delta_{1,i}(s)e^{-d_it}+\sum_{i=R}^{2R-1}\tau\epsilon_{1,i}(s)te^{-d_it}\right\}, \tag{26}$$

with

$$\delta_1(s)=\sum_{i=1}^{R-1}\frac{i\tau_i}{\tau}+g_0(s)\sum_{n=0}^{R-1}q_{n+R}s^n+\sum_{n=1}^{R-1}ng_{R-n}(s), \tag{27}$$

$$\delta_{1,n}(s)=\begin{cases}Rg_{R-n}(s)+g_0(s)\displaystyle\sum_{i=n}^{R-1}a_{i,n}s^i, & n=0,\ldots,R-1,\\ r_ns^{n-R}g_0(s), & n=R,\ldots,2R-1,\end{cases} \tag{28}$$

and

$$\epsilon_{1,n}(s)=p_ns^{n-R}g_0(s)/\tau,\quad n=R,\ldots,2R-1. \tag{29}$$

We now turn our attention to the generating function G_2. Introducing

$$G_1(s,t) = G_2(s,t) - \sum_{n=R}^{3R-1} N_n(t)s^n$$

into (22) gives

$$\frac{\partial G_2}{\partial t} + \tau s\frac{\partial G_2}{\partial s} = \tau\left[\gamma + \frac{s^R g_0(s)}{1-s}\right]G_2 + R_2(s,t), \quad (30)$$

where

$$R_2(s,t) = R_1(s,t) + \sum_{n=R}^{3R-1} s^n\left\{\frac{dN_n(t)}{dt} + \tau N_n(t)\left[n - \gamma - \frac{s^R g_0(s)}{1-s}\right]\right\}$$

or

$$R_2(s,t) = \sum_{n=R}^{3R-1}[(n-\gamma)\tau - d_{n-R}]s^n N_n(t) + \frac{s^{3R}}{1-s}\sum_{i=1}^{R-1} i\tau_i - \sum_{n=0}^{R-1} s^{n+2R}\sum_{i=0}^{n}(i+R)\tau_{n-i}$$
$$+ s^{2R}\sum_{n=0}^{R-1}\left\{\frac{\tau}{1-s}N_{n+R}(t)[s^R g_{R-n}(s) - s^n g_0(s)] + s^n\sum_{i=0}^{n}\tau_{n-i}N_{i+R}(t)\right\} + \sum_{n=0}^{2R-1} n d_n s^{n+R}, \quad (31)$$

where we used Eqs. (B2), (B5), and (25). Observing that the last sum but one on the rhs of Eq. (31) vanishes and taking into account Eqs. (10)–(12) and (14) yield

$$R_2(s,t) = \sum_{n=R}^{3R-2}\beta_n s^n N_n(t) + \frac{\phi(s)s^R}{1-s}, \quad (32)$$

where we put

$$\beta_n = (n-\gamma)\tau - d_{n-R}, \quad n = R,\ldots,3R-2, \quad (33)$$

and

$$\phi(s) = \sum_{i=1}^{R-1} s^i i\left[\tau_{i,0} + \tau_{0,i} + \sum_{n=1}^{R} s^n(\tau_{i,n} + \tau_{n,i} - \tau_{i,n-1} - \tau_{n-1,i})\right]. \quad (34)$$

Making once more use of (16) and (17) we finally see that

$$R_2(s,t) = \tau s^R\left\{\delta_2(s) + \sum_{n=0}^{2R-2}\delta_{2,n}(s)e^{-d_n t} + \sum_{n=R}^{2R-2}\tau\epsilon_{2,n}(s)te^{-d_n t}\right\}, \quad (35)$$

where

$$\tau\delta_2(s) = \sum_{n=1}^{R-1} n\beta_{n+R}s^n + \sum_{n=R}^{2R-2} q_n\beta_{n+R}s^n + \frac{\phi(s)}{1-s}, \quad (36)$$

$$\tau\delta_{2,n}(s) = \begin{cases} R\beta_{n+R}s^n + \sum_{i=n}^{R-2} a_{i,n}\beta_{i+2R}s^{i+R}, & n = 0,\ldots,R-1, \\ r_n\beta_{n+R}s^n, & n = R,\ldots,2R-2, \end{cases} \quad (37)$$

and

$$\epsilon_{2,n}(s) = p_n\beta_{n+R}s^n/\tau^2, \quad n = R,\ldots,2R-2. \quad (38)$$

V. CLOSED FORM SOLUTIONS FOR $\Theta(t)$

We now proceed to solve Eqs. (22) and (30). To this end, set

$$\xi(s) = \sum_{k=1}^{R-1}\frac{s^k}{k} + \sum_{k=R}^{2R-1}\frac{(1-\tau_{k-R}/2\tau)s^k}{k}, \quad (39)$$

and recall (23) to check that

$$2s(1-s)\xi'(s) = 2s - s^R g_0(s). \quad (40)$$

Owing to Eq. (40), substitution of

$$G_k(s,t) = (1-s)^{-2}s^\gamma e^{-2\xi(s)}H_k(s,t), \quad k = 1,2, \quad (41)$$

into

$$\frac{\partial G_k}{\partial t} + \tau s\frac{\partial G_k}{\partial s} = \tau\left[\gamma + \frac{s^R g_0(s)}{1-s}\right]G_k + R_k(s,t) \quad (42)$$

leads to the simpler equation

$$\frac{\partial H_k}{\partial t} + \tau s\frac{\partial H_k}{\partial s} = (1-s)^2 s^{-\gamma}e^{2\xi(s)}R_k(s,t), \quad k = 1,2. \quad (43)$$

Because of Eqs. (4)–(6) and (41) we must look for solutions satisfying the initial conditions

$$h_1(s) \equiv H_1(s,0) = e^{2\xi(s)}s^{3R-\gamma}[3R - (3R-1)s] \quad (44)$$

and

$$h_2(s) \equiv H_2(s,0) = e^{2\xi(s)}s^{R-\gamma}[R - (R-1)s]. \quad (45)$$

By tackling the auxiliary equations associated with (43) and using Eq. (26) we obtain, for $k = 1$,

$$H_1(s,t) = h_1(se^{-\tau t}) + f(se^{-\tau t}, s), \quad (46)$$

where

$$f(y,z)=\int_y^z (1-x)x^{\rho}\left\{\delta_1(x)+\sum_{i=0}^{2R-1}\left[\frac{y}{x}\right]^{d_i/\tau}\delta_{1,i}(x)+\sum_{i=R}^{2R-1}\left[\frac{y}{x}\right]^{d_i/\tau}\epsilon_{1,i}(x)\log\left(\frac{x}{y}\right)\right\}e^{2\xi(x)}\,dx.$$

Noting Eqs. (12) and (27)–(29) we see that $s^{\gamma}H_1(s,t)$ is (in the variable s), for any $t>0$, an integral function[19] of order at most $2R-1$. (It *is* of order $2R-1$ iff $\tau_{R-1}\neq 2\tau$.) Quite similar to former work[12,13] it therefore follows[19] from Eqs. (4), (41), and (43) [and on observing that $\xi'(1)=2R-2-\rho/2$], that for any $t>0$, $0<\epsilon<p=1/(2R-1)$, as $n\to\infty$,

$$N_n(t)=\left\{H_1(1,t)\left[n-R+\frac{\rho}{2}\right]+\frac{\partial H(1,t)}{\tau\,\partial t}\right\}e^{-2\xi(1)}+O(n^{-n(p-\epsilon)}). \tag{47}$$

Particularly,

$$1-\theta(t)=\lim_{n\to\infty}N_n(t)/n=H_1(1,t)e^{-2\xi(1)}, \tag{48}$$

or, more explicitly,

$$\theta(t)=1-e^{-2\xi(1)}\left\{h_1(e^{-\tau t})+\int_{e^{-\tau t}}^1(1-x)x^{\rho}\delta_1(x)e^{2\xi(x)}\,dx+\sum_{i=0}^{2R-1}e^{-d_i t}\int_{e^{-\tau t}}^1(1-x)x^{\rho-d_i/\tau}\delta_{1,i}(x)e^{2\xi(x)}\,dx\right.$$
$$\left.+\sum_{i=R}^{2R-1}e^{-d_i t}\int_{e^{-\tau t}}^1(1-x)x^{\rho-d_i/\tau}\epsilon_{1,i}(x)(\log x)e^{2\xi(x)}\,dx+\tau t\sum_{i=R}^{2R-1}e^{-d_i t}\int_{e^{-\tau t}}^1(1-x)x^{\rho-d_i/\tau}\epsilon_{1,i}(x)e^{2\xi(x)}\,dx\right\}. \tag{49}$$

Observe that Eq. (49) simplifies considerably if $\epsilon_{1,i}(x)\equiv 0$, $i=R,\ldots,2R-1$. Due to Eqs. (21) and (29), $\epsilon_{1,i}(x)\equiv 0$ whenever $d_i=0$ or when $d_j\neq d_i$, $j=0,\ldots,i-R$. Clearly, these conditions will be fulfilled in most cases.

Taking into account that $3R-\gamma=\rho+1>0$, we obtain from Eqs. (44) and (49) the following expression for the saturation coverage of an infinite lattice:

$$\theta^*=\lim_{t\to\infty}\theta(t)=1-e^{-2\xi(1)}\int_0^1(1-x)x^{\rho}\left[\delta_1(x)+\sum_{i\in M}\delta_{1,i}(x)\right]e^{2\xi(x)}\,dx, \tag{50}$$

where

$$M=\{i=0,1,\ldots,2R-1\,|\,d_i=0\}. \tag{51}$$

Similarly, a solution to Eq. (43), subject to the initial condition (45), may be found in the case $k=2$ and a relation analogous to Eq. (47) may be given. We desist from presenting the details and only state the following alternative representation of $\theta(t)$, based on Eqs. (36)–(38):

$$\theta(t)=1-e^{-2\xi(1)}\left\{h_2(e^{-\tau t})+\int_{e^{-\tau t}}^1(1-x)^2x^{\rho-2R}\delta_2(x)e^{2\xi(x)}\,dx+\sum_{n=0}^{2R-2}e^{-d_n t}\int_{e^{-\tau t}}^1(1-x)^2x^{\rho-2R-d_n/\tau}\delta_{2,n}(x)e^{2\xi(x)}\,dx\right.$$
$$+\sum_{n=R}^{2R-2}e^{-d_n t}\int_{e^{-\tau t}}^1(1-x)^2x^{\rho-2R-d_n/\tau}\epsilon_{2,n}(x)(\log x)e^{2\xi(x)}\,dx$$
$$\left.+\tau t\sum_{n=R}^{2R-2}e^{-d_n t}\int_{e^{-\tau t}}^1(1-x)^2x^{\rho-2R-d_n/\tau}\epsilon_{2,n}(x)e^{2\xi(x)}\,dx\right\}. \tag{52}$$

Clearly, Eq. (52) is valid for any $t\geqslant 0$. An asymptotic analysis, however, is problematic if $R-\gamma=1+\rho-2R<0$, since then integrals (if not identically vanishing) as well as $h_2(e^{-\tau t})$ diverge as $t\to\infty$. The following formula is therefore only true if $\rho-2R>-1$,

$$\theta^*=1-e^{-2\xi(1)}\int_0^1(1-x)^2x^{\rho-2R}\left[\delta_2(x)+\sum_{i\in M}\delta_{2,i}(x)\right]e^{2\xi(x)}\,dx, \tag{53}$$

with M as defined in Eq. (51).

For the purpose of numerical evaluation, Eq. (52) is, for obvious reasons, not suited if $\rho-2R<-1$ and t is large. However, if t and ρ become big, Eq. (49) must be treated with care, too.

Inspection of Eq. (52) [and the pertinent Eqs. (9), (11), (12), (18)–(21), (33), and (35)–(39)] shows that $\theta(t)$ does not depend on $\tau_{i,j}$ and $\tau_{j,i}$ separately but only on their sum $\tau_{i,j}+\tau_{j,i}$. A similar observation has been made formerly.[5,20]

As should be clear from our approach (see also comments in Sec. I and Appendix A) (49) and (52) *are* (different) *representations of a common value* [namely, $\theta(t)$], i.e., both representations [as well as (50) and (53)] reduce (necessarily) to a common form. In view of the complex formulas, to show this analytically (in a way different from

our "two-generating-function-approach") would be suicidal, however. Nevertheless, in the following consideration of special cases we find that there is consistency with earlier published results.

VI. EXAMPLES

Our most general R-mer filling with range-R cooperative effects described above includes the most different adsorption schemes, such as random filling, filling with nearest neighbor (range-R^*) effects, filling in stages, and filling with range-R^* blocking, $R^* \leqslant R$. Here we revisit some well-known cases and consider others not studied yet.

A. Random filling

In the case of random filling all rates are equal, i.e., $\tau_{i,j} = \tau$, $i,j \geqslant 0$. Consequently, $\tau_n = 2\tau$, $\rho = 2R$, $\gamma = R-1$, $d_n = (n+1)\tau$, and $\beta_n = 0$. Hence

$$\delta_{2,n}(s) = \epsilon_{2,n}(s) \equiv 0, \quad \xi(s) = \sum_{k=1}^{R-1} \frac{s^k}{k},$$

$$\delta_2(s) = \frac{\phi(s)}{\tau(1-s)} = 2\sum_{i=1}^{R-1} \frac{is^i}{1-s},$$

and we obtain from Eq. (52)

$$\theta(t) = 1 - e^{-2\xi(1)}\Big\{h_2(e^{-\tau t}) + 2\int_{e^{-\tau t}}^{1} (1-x)\sum_{i=1}^{R-1} ix^i e^{2\xi(x)}\,dx\Big\}. \quad (54)$$

The saturation coverage is therefore of the form[10,11]

$$\theta^* = 1 - 2e^{-2\xi(1)}\int_0^1 (1-x)\sum_{i=1}^{R-1} ix^i e^{2\xi(x)}\,dx. \quad (55)$$

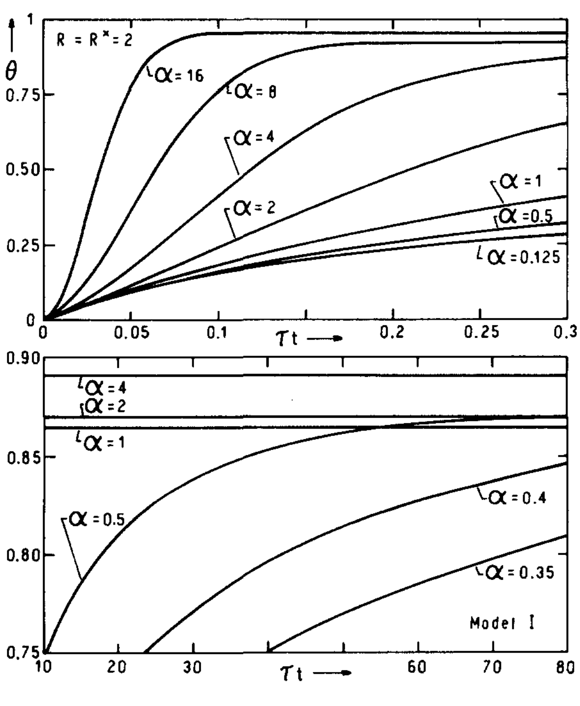

FIG. 1. The lattice coverage $\theta(\alpha,\tau t)$ as function of τt for various values of α in the case of dimer filling with model I range-2 cooperative effects (see Sec. VI D).

An alternative representation of θ^* has first been given by Mackenzie[9] (see also Appendix C). Another one will be obtained in Sec. VI B below.

In Figs. 1 and 2 (Figs. 3 and 4) the $\alpha = 1$ case corresponds to random dimer (trimer) filling.

B. Range-R^* blocking

R-mer filling with range R^* blocking,[1] $0 < R^* < R$, requires

$$\tau_{i,j} = \begin{cases} \tau, & \text{if } i,j \geqslant R^*, \\ 0, & \text{otherwise,} \end{cases}$$

i.e., the rate matrix $(\tau_{i,j})$ has the following form (remember that $i,j = 0,1,\ldots$):

$$(\tau_{i,j}) = \begin{pmatrix} 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & \\ 0 & 0 & & 0 & 0 & 0 & 0 & \cdots \\ 0 & 0 & \cdots & 0 & \tau & \tau & \tau & \cdots \\ 0 & 0 & \cdots & 0 & \tau & \tau & \tau & \cdots \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & \end{pmatrix}$$

(the first R^* columns and the first R^* rows are zero).

Then

$$\tau_j = \begin{cases} 0, & j = 0,\ldots,R^*-1, \\ 2\tau, & j = R^*,\ldots,R-1, \end{cases}$$

$$\rho = 2(R - R^*), \quad \gamma = R + 2R^* - 1,$$

$$d_n = \begin{cases} 0, & n = 0,\ldots,2R^*-1, \\ (n - 2R^* + 1)\tau, & n = 2R^*,\ldots,2R-1, \end{cases}$$

$$g_k(s)\begin{cases} 2s^{R^*-k}, & k = 0,\ldots,R^*, \\ 2, & k = R^*+1,\ldots,R-1, \end{cases}$$

$$\xi(s) = \sum_{k=1}^{R+R^*-1} \frac{s^k}{k}, \quad \epsilon_{1,n}(s) \equiv 0, \quad n = R,\ldots,2R-1,$$

and expressions for q_n, r_n, and $a_{n,i}$, and hence for δ_1 and $\delta_{1,n}$, follow easily. Rather than to state these explicitly for general R^* we confine ourselves to illustrate two cases: $R^* = R$ and $R^* = 0$.

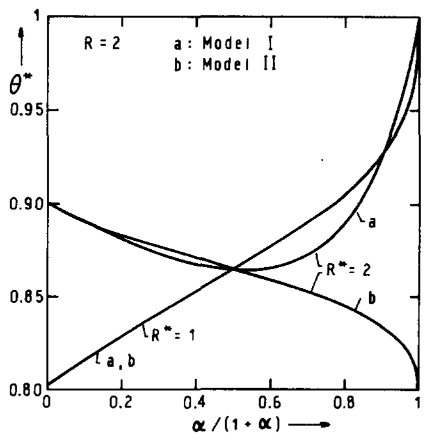

FIG. 2. The saturation coverage θ^* for dimer filling with model I and model II range-R^* cooperative effects. $R^* = 1,2$ are shown.

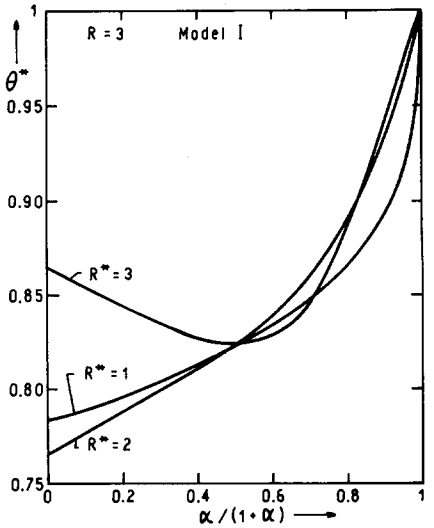

FIG. 3. The saturation coverage θ^* for trimer filling with model I range-R^* cooperative effects. $R^* = 1,2,3$ are shown.

(i) For range-R blocking

$$\delta_1(s) = 2\sum_{n=1}^{R-1} ns^n$$

and

$$\delta_{1,n}(s) = \begin{cases} 2Rs^n, & n = 0,\ldots,R-1, \\ 2(n+R)s^n, & n = R,\ldots,2R-1. \end{cases}$$

Equation (49) therefore yields

$$\theta(t) = 1 - e^{-2\xi(1)}\left\{h_1(e^{-\tau t}) + 2\int_{e^{-\tau t}}^1 (1-x)\sum_{n=0}^{2R-1}(n+R)x^n e^{2\xi(x)}\,dx\right\}$$

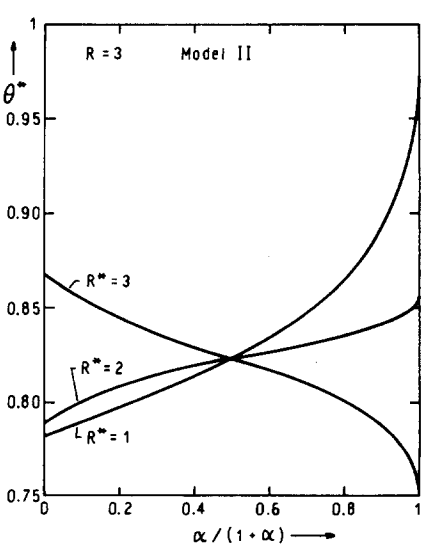

FIG. 4. The saturation coverage θ^* in the case of trimer filling with model II range-R^* cooperative effects. $R^* = 1,2,3$ are shown.

and

$$\theta^* = 1 - 2e^{-2\xi(1)}\int_0^1 (1-x)\sum_{n=0}^{2R-1}(n+R)x^n e^{2\xi(x)}\,dx. \tag{56}$$

We cross-check Eq. (56) by means of an isomorphism argument in Appendix C.

(ii) For range-0 blocking, i.e., random filling, it is seen that

$$\theta^* = 1 - 2e^{-2\xi(1)}\int_0^1 (1-x)x^{2R}\left\{R(R-1) + \sum_{n=0}^{R-1} x^n\left[n+R-\frac{2R(n+1)}{n+R+1}\right]\right\}e^{2\xi(x)}\,dx. \tag{57}$$

Observe that it would be extremely tedious to prove the equality of the representations (55) and (57) by common methods (integration by parts, etc.).

Some numerical values for R-mer filling with range-R^* blocking ($R = 1,\ldots,7$) may be found in Ref. 1.

C. Nearest neighbor cooperative effects

Here the rate matrix $(\tau_{i,j})$ is of the form

$$(\tau_{i,j}) = \begin{pmatrix} \sigma_0 & \sigma_1 & \sigma_1 & \cdots \\ \sigma_1' & \tau & \tau & \cdots \\ \sigma_1' & \tau & \tau & \cdots \\ \vdots & \vdots & \vdots & \end{pmatrix}.$$

We remark that rates with reflection unsymmetry (here the case $\sigma_1' \neq \sigma_1$) have been considered earlier.[5,20,21] To simplify notation, set $2K = \tau_0/\tau$, $L = \sigma_0/\tau$, and $\alpha = e^{-\tau t}$. For the variables pertinent to Eq. (52) we then find

$$\rho = 2(R-1+K), \quad \tau_0 = \sigma_1 + \sigma_1'$$

and

$$d_n = \begin{cases} \sigma_0, & n = 0 \\ \tau_0 + (n-1)\tau, & n = 1,2,\ldots\ . \end{cases}$$

Owing to the fact that $\beta_n = 0$, $n = R+1,\ldots,$

$$\epsilon_{2,n}(s) \equiv 0$$

and

$$\delta_{2,n}(s) = \begin{cases} R(2K-L-1), & n = 0, \\ 0, & n = 1,2,\ldots,2R-2, \end{cases}$$

and Eq. (52) therefore simplifies significantly:

$$\theta(t) = 1 - e^{-2\xi(1)}\left\{h_2(\alpha) + \frac{1}{\tau}\int_\alpha^1 (1-x)x^{2K-2}\phi(x)e^{2\xi(x)}\,dx + R(2K-L-1)\alpha^L\int_\alpha^1 (1-x)^2 \times x^{2K-L-2}e^{2\xi(x)}\,dx\right\}, \tag{58}$$

where

$$\xi(s) = \sum_{k=1}^{R-1}\frac{s^k}{k} + \frac{s^R(1-K)}{R}$$

and

$$\phi(s) = [2\tau - \tau_0](R-1)s^R + \sum_{k=1}^{R-1} [\tau_0 + 2\tau(k-1)]s^k.$$

The case $\sigma_0 = \sigma_1 = \sigma_1' = \tau$ corresponds to random filling. Then, but also (we commented on this fact at the end of Sec. V) when $\sigma_0 = \tau$, $\tau_0 = \sigma_1 + \sigma_1' = 2\tau$, $\sigma_1 \neq \sigma_1'$, Eqs. (54) and (58) coincide. Range-1 blocking is obtained for $\sigma_0 = \sigma_1 = \sigma_1' = 0$.

Former analysis of nearest neighbor effects[4,6] dealt with sequence distributions, thus providing expressions for $\theta(t)$ via Eq. (1). A direct comparison of these results with our comparatively compact expression (58) is somewhat cumbersome (at least if $R \geq 2$).

For monomer filling with nearest neighbor cooperative effects, $\phi(x) \equiv 0$ and only one integral term is retained in Eq. (58). Recalling (45) and carrying out an integration by parts gives

$$\theta(t) = 1 - e^{-2\xi(1)}\left\{(2-\alpha)\alpha^{2K}e^{2\xi(\alpha)} + 2\alpha^L \int_\alpha^1 x^{2K-L-1} \times [K(1-x)^2 + x(1-x)]e^{2\xi(x)}\,dx\right\}, \tag{59}$$

which is Eq. (3.2) of Boucher.[16] Passing to the limit $t \to \infty$ in Eq. (59) provides, when $L = 0$, i.e., $\sigma_0 = 0$,

$$\theta^* = 1 - 2e^{-2\xi(1)} \int_0^1 x^{2K-1}[K(1-x)^2 + x(1-x)]e^{2\xi(x)}\,dx.$$

In the same case ($R = 1, L = 0$), Eq. (58) yields, on assuming $K > \frac{1}{2}$, the alternative expression

$$\theta^* = 1 - e^{-2\xi(1)}(2K-1)\int_0^1 (1-x)^2 x^{2K-2} e^{2\xi(x)}\,dx.$$

In the general case, $R \geq 1$, but if $K > \frac{1}{2}$ and $L > 0$, we obtain, from Eq. (58),

$$\theta^* = 1 - (1/\tau)e^{-2\xi(1)} \int_0^1 (1-x)x^{2K-2}\phi(x)e^{2\xi(x)}\,dx.$$

To get an expression for θ^* in the case $K \leq \frac{1}{2}$ one may utilize Eq. (50).

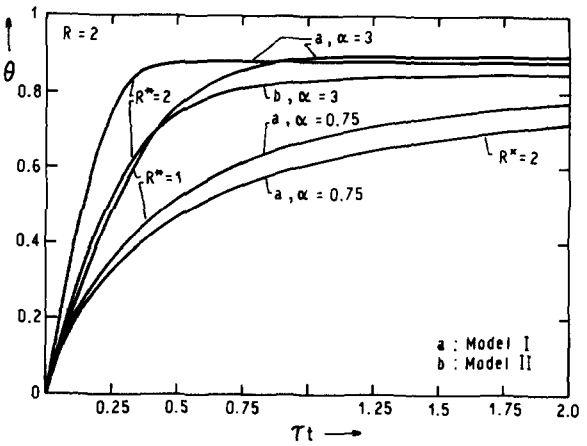

FIG. 5. The lattice coverage $\theta(\alpha, \tau t)$ as function of τt for $\alpha = 3$ and $\alpha = 0.75$ in the case of dimer filling with model I and model II range-R^* cooperative effects (see Secs. VI D and VI F). $R^* = 1,2$ are shown.

In Figs. 2–5 the case $R^* = 1$ corresponds to nearest neighbor effects. In model I (see Refs. 1 and 6),

$$\sigma_0 = \alpha^2\tau \quad \text{and} \quad \sigma_1 = \sigma_1' = \alpha\tau,$$

i.e., each filled nearest neighbor changes the rate by a factor α. In model II, the effect of two filled nearest neighbors is assumed to be equal to that of one alone, i.e.,

$$\sigma_0 = \sigma_1 = \sigma_1' = \alpha\tau.$$

We discuss these models in more detail in the following sections.

D. Model I

Let $1 < R^* < R$. The adsorption scheme associated with the rate matrix

$$(\tau_{i,j}) = \begin{pmatrix} \tau\alpha^{2R^*} & \tau\alpha^{2R^*-1} & \cdots & \tau\alpha^{R^*+1} & \tau\alpha^{R^*} & \tau\alpha^{R^*} & \cdots \\ \tau\alpha^{2R^*-1} & \tau\alpha^{2R^*-2} & \cdots & \tau\alpha^{R^*} & \tau\alpha^{R^*-1} & \tau\alpha^{R^*-1} & \cdots \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \\ \tau\alpha^{R^*+1} & \tau\alpha^{R^*} & \cdots & \tau\alpha^2 & \tau\alpha & \tau\alpha & \cdots \\ \tau\alpha^{R^*} & \tau\alpha^{R^*-1} & \cdots & \tau\alpha & \tau & \tau & \cdots \\ \tau\alpha^{R^*} & \tau\alpha^{R^*-1} & \cdots & \tau\alpha & \tau & \tau & \cdots \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \end{pmatrix}$$

will be called model I (with range-R^* cooperative effects). Here each filled site—within range R^*—modifies the basic rate τ by a factor α. For $R^* = 1$ this rate regime has been considered previously.[1,6,22] Observe that the $\alpha = 1$ case corresponds to random filling and the case $\alpha = 0$ to range-R^* blocking.

Here

$$\rho = 2\left(R - R^* + \sum_{i=1}^{R^*} \alpha^i\right) = 3R - 1 - \gamma$$

and

$$\frac{d_n}{\tau} = \begin{cases} (n+1)\alpha^{2R^*-n}, & n = 0,1,\ldots,R^*-1, \\ 2\sum_{i=2R^*-n}^{R^*} \alpha^i + (2R^* - n - 1)\alpha^{2R^*-n}, & \\ \qquad n = R^*,\ldots,2R^*-2, & \\ 2\sum_{i=1}^{R^*} \alpha^i + (n - 2R^* + 1)\tau, & \\ \qquad n = 2R^*-1,\ldots,2R-1. & \end{cases}$$

Hence $\beta_n = 0$ for all $n > 2R^* - 1 + R$ and therefore

$$\delta_{2,n}(s) \equiv 0 \equiv \epsilon_{2,n}(s), \quad \text{for } n > 2R^* - 1.$$

In consequence, the summation index n in Eq. (52) runs only up to $2R^* - 2$.

Clearly, $\theta(t)$ may be expressed explicitly in terms of only R, R^*, α, τ, and t, but such efforts do not lead to an apparent simplification of Eqs. (49) and (52). We therefore desist from doing this. We only remark that, given τ and $n < 2R^* - 2$, there are generally α-values such that $d_i = d_{n+R}$ for some $i = 0,\ldots,n$ [see Eq. (21)]. Hence [see Eqs. (29) and (38)] integrals involving the logarithmic function may contribute [Eqs. (49) and (52)] for $\theta(t)$.

The dependence of $\theta = \theta(\alpha,\tau t)$ on τt, for various values of α, is shown in Fig. 1 in the case of dimer filling with range-2 cooperative effects. For autocatalytic rates, i.e., $\alpha > 1$, θ is—in some neighborhood of zero—a convex function. Thus, as to be expected, adsorption accelerates only after an induction period[23] in which filling is governed almost exclusively by the (initiation) rate τ. Further observe that high autocatalytic rates lead to an almost instantaneous lattice saturation *but not necessarily* to a saturation coverage that exceeds the saturation value of any autoinhibitory rate regime. For example, for $\alpha = 2$, filling comes to an end [the saturation value is $\theta^*(2) = 0.8699$] at time $\tau t = 1.7$ approximately. At this moment the adsorption process with $\alpha = 0.5$ arrives at only 64% of its saturation value $\theta^*(0.5) = 0.8709$, which, nevertheless, is greater than $\theta^*(2)$. Equality of coverages is achieved at about $\tau t = 86$, i.e., $\theta(0.5,86) = \theta(2,86)$. This may be appreciated (partially) in Fig. 1. In Fig. 2 we have shown the saturation coverage θ^* as function of $\alpha/(1+\alpha)$. Note the curious fact that random filling ($\alpha = 1$) produces the least saturation coverage. The curve corresponding to range-1 cooperative effects ($R^* = 1$) has been shown in Ref. 1, too. In Fig. 3, saturation coverages are shown for trimer filling with range-R^* cooperative effects, $R^* = 1,2,3$. Realize that autoretardative rate regimes exhibit extraordinarily high saturation values only if cooperative effects are effectively of range $R^* = 3$.

This somewhat strange-looking (and up to our knowledge not formerly observed) behavior of model I R-mer filling with range-R cooperative effects is due to occupational degeneracies of small-size gaps. As an example, we consider (model I) dimer filling and compare range-1 with range-2 cooperative effects for a small α regime. It is the filling of 4- and 6-gaps that exhibits fundamental differences (2-, 3- and 5-gaps show equal saturation values in both adsorption schemes): If $R^* = 2$ all three doublets of a 4-gap become occupied with equal rate $\alpha^2\tau$; on the average 2/3 sites remain therefore finally empty. If $R^* = 1$ the middle doublet (rate τ) is much more active than its two neighbor doublets (rates $\alpha\tau$, $\alpha \ll 1$); hence, at the end, almost surely two units remain unoccupied. As to a 6-gap, the situation is similar. For $R^* = 2$ the middle doublet becomes occupied first (its rate τ dominates over the competing rates $\tau\alpha$ and $\tau\alpha^2$) and the originating 2-gaps become filled later. If $R^* = 1$, only the second, third, and fourth doublets compete for a first adsorption (with equal rate τ); winning the second or third, two sites (of the initial 6-gap) will finally remain empty, i.e., 4/3 on the average. In summary, range-2 cooperative effects exploit space much better than range-1 cooperative effects do. Similar considerations apply to trimer filling (Fig. 3), to weak autocatalytic (anticooperative) effects, i.e., $\alpha \simeq 1$, and to high α regimes. In the latter case, R-mers grow about a nucleating R-mer to form an island.[1,17] Clearly, imperfections in island formation (holes) are less probable in the case of range-R cooperative effects; then an R-tuplet next to (touching) the island becomes occupied with rate $\tau\alpha^R$, which is to be compared with the (much smaller) rate $\tau\alpha^{R^*}$ if cooperative effects are restricted to range $R^* < R$. This explains the behavior of θ^* (Figs. 2 and 3) for $\alpha \to \infty$.

E. Model II

While in model I *each* filled site—within the influencing environment of width R^*—contributes to a rate modification, in model II a change in the adsorption rate will be due only to the existence or nonexistence of filled neighboring sites (independent of their number). More precisely, it will be assumed that the basic rate τ is changed by a factor α if at least one unit—within range $R^* \leqslant R$—is filled, i.e.,

$$(\tau_{i,j}) = \begin{pmatrix} \overbrace{\alpha\tau & \alpha\tau & \cdots & \alpha\tau}^{R^*} & \alpha\tau & \alpha\tau & \cdots \\ \alpha\tau & \alpha\tau & \cdots & \alpha\tau & \alpha\tau & \alpha\tau & \cdots \\ \vdots & \vdots & & \vdots & \vdots & & \\ \alpha\tau & \alpha\tau & \cdots & \alpha\tau & \alpha\tau & \alpha\tau & \cdots \\ \alpha\tau & \alpha\tau & \cdots & \alpha\tau & \tau & \tau & \cdots \\ \alpha\tau & \alpha\tau & \cdots & \alpha\tau & \tau & \tau & \cdots \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \end{pmatrix} \Big\} R^*.$$

If $R^* = 1$ only the adsorption rates of R-gaps differ in models I ($\alpha^2\tau$) and II ($\alpha\tau$). This causes slight differences in the time behavior of the respective lattice coverages (differences are so tenuous that they would be hardly visible in Fig. 5) but the saturation coverages of both models clearly coincide (see Figs. 2–4).

For dimer filling with range-2 cooperative effects, models I and II behave quite differently in the $\alpha \to \infty$ limit (Fig. 2). Whereas, in model I, a saturation coverage of unity is achieved by perfect island formation,[1,17] in model II island formation is "imperfect" (full of holes) and $\frac{1}{3}$ of the lattice remains finally empty. Clearly, in model II, the two doublets next to an (actual) end of the "island" have equal rates $\tau\alpha$ and compete with each other for adsorption (such a compe-

tition does not exist in model I since rates are rather unlike: $\tau\alpha^2 \gg \tau\alpha$). Thus, half of the dimers will not stick close to the "island" but will leave a one-unit hole. An easy method [not relying upon Eqs. (50) or (53)] to determine $\theta^*(\infty) = \lim_{\alpha\to\infty} \theta^*(\alpha)$ is the following. Consider a linear lattice of n sites. First, put a dimer on sites 1–2–3 at random. If it landed on sites 1–2 (2–3) place a second dimer on sites 3–4–5 (4–5–6) randomly. Continue in this way until the lattice is saturated and call the average number of finally unoccupied sites a_n. Then $a_1 = 1$, $a_2 = 0$, $a_3 = 1$, and $a_n = \frac{1}{2}(1 + a_{n-3} + a_{n-2})$, $n = 4,5,\ldots$. Furthermore,

$$1 - \theta^*(\infty) = \lim_{n\to\infty} a_n/n = \tfrac{1}{3}.$$

Similar recursion relationships may be derived for any $1 \leqslant R^* \leqslant R$. We only state two further results. For $R = 3$ (see Fig. 4),

$$\lim_{\alpha\to\infty} \theta^*(\alpha) = \begin{cases} \frac{6}{7}, & \text{if } R^* = 2, \\ \frac{3}{4}, & \text{if } R^* = 3. \end{cases}$$

F. Filling in stages

The limiting rate regime of R-mer filling in stages[1,2,7,24] can be solved exactly for range-R^* (arbitrary) cooperative effects. This has been shown in Ref. 1 where the case of monomer filling (in stages) is treated in detail. Here we consider R-mer filling occurring in $2R^* + 1$ ($R^* \leqslant R$) stages, consecutively, with no filled sites in the cooperative range R^*, with just one [$(R + 2R^* - 1)$-gap], then two [$(R + 2R^* - 2)$-gap] filled R^*th nearest neighbors, etc. Clearly, this occupation procedure is the $\alpha\downarrow 0$ limit of model I with range-R^* cooperative effects. Calling the respective saturation coverage $\theta_1^*(R^*,R)$ we obtain from Sec. VI D and Eq. (50)

$$\theta_1^*(R^*,R) = 1 - 2e^{-2\xi(1)} \int_0^1 (1-x)x^\rho \times \left[R(R-R^*) + \sum_{i=1}^{R^*-1} (R - R^* + i)x^i + x^{R^*} \sum_{n=0}^{R-1} q_{n+R} x^n \right] e^{2\xi(x)}\, dx, \tag{60}$$

where

$$\rho = 2(R - R^*), \quad \xi(s) = \sum_{k=1}^{R+R^*-1} \frac{s^k}{k},$$

$$q_n = \begin{cases} n, & n = R,\ldots,R + R^* - 1, \\ n - \dfrac{2R(n - R - R^* + 1)}{n - 2R^* + 1}, & n = R + R^*,\ldots,2R - 1, \end{cases}$$

$$R = R^* + 1, R^* + 2,\ldots, \quad R^* = 1,2,\ldots,$$

and, in the case $R = R^*$,

$$q_n = n - 2R/(2R + 1 - n), \quad n = R,\ldots,2R - 1.$$

In Table I, we catalog $\theta_1^*(R^*,R)$ for $R^* = 1,\ldots,R$, $R = 2,\ldots,8$.

The $\alpha\downarrow 0$ limit of model II with range-R^* cooperative effects corresponds to R-mer filling in two stages. In the first stage (identical to the first filling step in the above-described model) only R-tuplets with no filled sites in the cooperative range R^* become (randomly) occupied, i.e., filling terminates when only R-, $(R + 1)$-,...,$(R + 2R^* - 1)$-gaps remain. These, in the second stage, are then filled *randomly*. Denoting the thus-arising saturation coverage by $\theta_2^*(R^*,R)$ we observe that differences between $\theta_1^*(R^*,R)$ and $\theta_2^*(R^*,R)$ are due only to different filling of $2R$-, $(2R + 1)$-,..., $(R + 2R^* - 1)$-gaps. Particularly, if $2R^* + 1 < R$, then $\theta_1^*(R^*,R) = \theta_2^*(R^*,R)$. If $2R^* - 1 \geqslant R$, then $\theta_1^*(R^*,R) < \theta_2^*(R^*,R)$ since the deterministic filling [in the second, third,...,$(2R^* + 1)$st stage] of model I does not admit close packing whereas the random filling (in the second stage) of model II certainly does. A comparison of Tables I and II [in the latter are shown $\theta_2^*(R^*,R)$, $R^* = 1,\ldots,R$, $R = 2,\ldots,8$] corroborates these considerations. Clearly, a closed form expression for $\theta_2^*(R^*,R)$ [very similar to that of $\theta_1^*(R^*,R)$] is easily obtainable from Eq. (50) and therefore will not be stated.

VII. DISCUSSION

By means of a generating function technique we have studied the kinetics of R-mer filling with general range-R cooperative effects. The exact closed form expression for the lattice coverage obtained here embraces formerly gotten ex-

TABLE I. Saturation coverages $\theta_1^*(R^*,R)$ for R-mer filling in $2R^* + 1$ stages ($\alpha\downarrow 0$ limit of model I with range-R^* cooperative effects); see Eq. (60).

R^*	1	2	3	4	5	6	7	8
$R = 2$	0.8022	0.9009						
$R = 3$	0.7829	0.7656	0.8639					
$R = 4$	0.7737	0.7557	0.7520	0.8433				
$R = 5$	0.7682	0.7518	0.7434	0.7456	0.8298			
$R = 6$	0.7647	0.7499	0.7404	0.7369	0.7421	0.8202		
$R = 7$	0.7622	0.7489	0.7393	0.7338	0.7333	0.7401	0.8129	
$R = 8$	0.7603	0.7483	0.7390	0.7327	0.7298	0.7311	0.7390	0.8070

TABLE II. Saturation coverages $\theta_2^*(R^*,R)$ for R-mer filling in two stages ($\alpha\downarrow 0$ limit of model II with range-R^* cooperative effects).

R^*	1	2	3	4	5	6	7	8
$R=2$	0.8022	0.9009						
$R=3$	0.7829	0.7888	0.8689					
$R=4$	0.7737	0.7557	0.7857	0.8531				
$R=5$	0.7682	0.7518	0.7527	0.7851	0.8437			
$R=6$	0.7647	0.7499	0.7404	0.7540	0.7854	0.8375		
$R=7$	0.7622	0.7489	0.7393	0.7387	0.7563	0.7859	0.8331	
$R=8$	0.7603	0.7483	0.7390	0.7327	0.7402	0.7588	0.7867	0.8299

plicit results for R-mer filling with nearest neighbor cooperative effects.[4,6,16,18]

Figures 1 and 5 reveal that the kinetic behavior of range-R cooperative processes is—for short times—quite similar to that of filling processes with nearest neighbor cooperative effects.[6,16,18] However, the law (valid for nearest neighbor cooperative effects) that "anticooperative rate regimes lead to a *lower* saturation level since R-mers tend to avoid each other, leaving gaps that cannot be filled[6]" is no longer true for genuine range-R cooperative effects (see Figs. 1–4).

The kinetics of an irreversible process, where R_1-, R_2-, ..., and R_r-mers (with relative frequencies $p_1 \geqslant 0$, $p_2 \geqslant 0$,..., and $p_r > 0$, respectively) are placed *randomly* onto a linear lattice, has been considered recently.[13] An analysis of the more general problem, where occupation occurs *cooperatively*, seems to be much more involved. However, certain related problems such as competition between different monomer types on homogeneous[3] and nonuniform[21] (e.g., periodic and stochastic copolymers) lattices and special cases of competition between monomers and dimers[3] have been treated successfully.

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APPENDIX A: A NOTE ON THE GENERATING FUNCTION TECHNIQUE

Here we illustrate the "nonuniqueness"of the generating function approach by means of a simple example (which corresponds to random dimer filling; b_n denotes the number of empty sites in a $1\times n$ lattice). Given the difference equation

$$(n-1)b_n - (n-2)b_{n-1} = 2b_{n-2}, \quad n = 3,4,..., \tag{A1}$$

with initial conditions

$$b_1 = 1, \quad b_2 = 0, \tag{A2}$$

we want to know the behavior of b_n as $n\to\infty$. Since (A1) is valid for $n = 3,4,...$, it appears to be convenient to introduce the generating function

$$A(s) = \sum_{n=3}^{\infty} b_n s^{n-1}. \tag{A3}$$

With this choice (A1) becomes

$$A'(s) - [2s/(1-s)]A(s) = 2s/(1-s),$$

which is to be solved subject to the condition $A(0) = 0$. We find

$$A(s) = 2(1-s)^{-2}\int_0^s (1-t)te^{2(t-s)}\,dt$$

and hence

$$b \equiv \lim_{n\to\infty}\frac{b_n}{n} = 2\int_0^1 (1-t)te^{2(t-1)}\,dt. \tag{A4}$$

The proposed task is thus accomplished. However, the choice in (A3) is arbitrary (i.e., we could have defined the generating function in any other way) and a natural question arises: Would another definition have led to a different result? Obviously, the numerical value of b [which is uniquely determined by the recursion relation (A1) together with the initial condition (A2)] cannot depend on the choice of the generating function. But what may depend on the specific form of the generating function is the *representation* of b (i.e., the algebraic expression giving b). To explore such a possibility let us try, for example,

$$B(s) = \sum_{n=1}^{\infty} b_n s^{n-1}. \tag{A5}$$

With this definition, (A1) is converted into the homogeneous equation

$$B'(s) - [2s/(1-s)]B(s) = 0,$$

whose solution, satisfying $B(0) = 1$, is given by

$$B(s) = (1-s)^{-2}e^{-2s}.$$

Hence

$$b = e^{-2}. \tag{A6}$$

This shows that different choices of the generating function [here (A3) and (A5)] will generally lead to *different* representations [here (A4) and (A6), respectively] of the *same* object (namely, $b \equiv \lim_{n\to\infty} b_n/n$). We emphasize the fact that the equality of (different) representations is given *a priori* and must not be proved *a posteriori*. Thus, in the present example, the equality of the expressions on the right-hand sides of (A4) and (A6) holds true without further proof.

Since different representations may be rather unlike [compare (A4) with (A6)] it is always worthwhile to look for that generating function (this is by trial and error) that is accompanied by the most appropriate (simple) representation. Clearly, one could work with a single generating function [e.g., that introduced in (A3)] and try to transform (if necessary and/or desirable) the corresponding representation [e.g., evaluate the integral in (A4)]. However, labor thus involved is generally so heavy that it is more advantageous to introduce changes in the definition of the generating function and to examine the effects on the associated representations. Such an approach has been used successfully[10,11] and proves to be most helpful in the present paper, too.

APPENDIX B: DERIVATION OF RATE EQUATIONS

Recall Eqs. (10) and (11), let $n \geqslant R$, and consider a lattice of $n+2R$ sites (as described in Sec. II). Due to our boundary condition there are initially $n-R+1$ R-tuplets. Numbering these from left to right, $0,1,\ldots,n-R$, we observe that the occupation of a *first* R-tuplet, the jth, say, subdivides the lattice into two sublattices (of j and $n-R-j$ empty sites), which are subsequently subject to further filling under the *same* boundary condition as the original lattice was, i.e., the R sites on both their ends belong to—and only to—the influencing environment of neighboring sequences of R filled sites. (Note that this affirmation would not be true if cooperative effects were of range $R^* > R$.) Since, within the time interval $(0,h)$, the just-considered event occurs with probability $\tau_{j,n-R-j}h + o(h)$ and since "nothing" happens with probability $1 - d_{n-R}h + o(h)$ it therefore follows that

$$N_n(t+h) = (1 - d_{n-R}h)N_n(t) + h\sum_{j=0}^{n-R}(\tau_{j,n-R-j} + \tau_{n-R-j,j})N_j(t) + o(h)$$

or

$$\frac{dN_n(t)}{dt} = -d_{n-R}N_n(t) + \sum_{j=0}^{n-R}(\tau_{j,n-R-j} + \tau_{n-R-j,j})N_j(t), \quad n \geqslant R. \tag{B1}$$

On observing Eqs. (7)–(11) and (13), Eq. (B1) becomes

$$\frac{dN_{n+R}(t)}{dt} = -d_n N_{n+R}(t) + nd_n, \quad n = 0,1,\ldots,R-1, \tag{B2}$$

$$\frac{dN_{n+2R}(t)}{dt} = -d_{n+R}N_{n+2R}(t) + \sum_{i=0}^{n}\tau_{n-i}(N_{i+R}(t) - i - R) + (n+R)d_{n+R}, \quad n = 0,1,\ldots,R-1, \tag{B3}$$

and reduces to (15) for $n = 3R-1, 3R, \ldots$. The solution to (B2), obeying the initial condition (6), is

$$N_{n+R}(t) = n + Re^{-d_n t}, \quad n = 0,1,\ldots,R-1. \tag{B4}$$

Introducing (B4) into Eq. (B3) gives

$$\frac{dN_{n+2R}(t)}{dt} = -d_{n+R}N_{n+2R}(t) + (n+R)d_{n+R} - R\sum_{i=0}^{n}\tau_i + R\sum_{i=0}^{n}\tau_{n-i}e^{-d_i t}. \tag{B5}$$

Imposing the initial condition (6), Eq. (B5) yields (17).

APPENDIX C: *R*-MER FILLING WITH RANGE-*R* BLOCKING

As pointed out by a referee, R-mer filling with range-R blocking is isomorphic to $2R$-mer random filling (see also Ref. 1). This observation permits a cross-check on Eq. (56). From the scheme [where $R = 2$ and where 1's (0's) represent occupied (empty) sites]

...00110000011000011000011001100...
....11110001111001111011111111... ,

we learn that

$$2\theta^* = \theta', \tag{C1}$$

where θ' denotes the saturation coverage for $2R$-mer random filling. Now, from (55),

$$\theta' = 1 - 2e^{-2\xi(1)}\int_0^1 (1-x)\sum_{n=0}^{2R-1} nx^n e^{2\xi(x)}\,dx. \tag{C2}$$

On the other hand, from Eqs. (40) and (41) of Ref. 11,

$$\theta' = 2Re^{-2\xi(1)}\int_0^1 e^{2\xi(x)}\,dx \tag{C3}$$

and

$$\theta' = 4Re^{-2\xi(1)}\int_0^1 x^{2R}e^{2\xi(x)}\,dx, \tag{C4}$$

respectively. Subtracting $\theta'/2$ [in the form given by Eq. (C4)] from (C3) gives

$$\theta'/2 = 2Re^{-2\xi(1)}\int_0^1 (1-x^{2R})e^{2\xi(x)}\,dx = 2Re^{-2\xi(1)}\int_0^1 (1-x)\sum_{n=0}^{2R-1} x^n e^{2\xi(x)}\,dx. \tag{C5}$$

Finally, on subtracting (C5) from (C2) and on observing (C1) we recover (56). Note that it is a somewhat tricky exercise to prove the equality of representations (C2)–(C4) by methods of integration.

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On the phase transition of the three-dimensional Percus–Yevick equation for an arbitrary potential of finite range

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A qualitative study of the three-dimensional Percus–Yevick (PY) equation by means of Baxter's relations is considered for an arbitrary potential of finite range l by a perturbation method. It is shown that the PY equation has a unique solution $Y(r,\eta,\beta\S)$ and a unique solution $Q(r,\eta,\beta\S)$ if the following conditions are satisfied: (i) $0<\eta<0.175$, (ii) $0<\beta\S<(\beta\S)_0$, (iii) $\mathrm{Sup}_{r\in[0,l]}|Q_n|<n!$ and $\mathrm{Sup}_{r>0}|Y_n(r)|<n!$, where both Q and Y are continuous functions of the reduced density η, and can expressed as absolutely and uniformly convergent series $Y=\Sigma_{n=0}^{\infty}(1/n!)(\beta\S)^n Y_n(r,\eta)$, $Q=\Sigma_{n=0}^{\infty}(1/n!)(\beta\S)^n Q_n(r,\eta)$ within the radius of convergence of the inverse reduced temperature $(\beta\S)_0$. As functions of r, $Q\in C^{(0)}[0,l]$ with $Q(l)=0$, whereas Y is continuous for $r\geqslant 0$ except for a possible finite discontinuity at $r=1$, and $Y-r\to 0$ exponentially as $r\to\infty$. Based on the solution of Y and Q, the isothermal compressibility $K_T=KT(\partial\rho/\partial P)_T$ is a continuous and bounded function of η. As $\eta\to\eta_c=0.175$, K_T becomes divergent. The critical density η_c (or ρ_c) is independent of the range of the attractive potential l. On the other hand, the critical temperature $(\beta\S)_c$ is determined by the positive root of $F(\beta\S)=12\eta\int_0^l Q(r)dr=1$, which depends explicitly on the value of l.

I. INTRODUCTION

Consider a classical system of N molecules in a volume V and at temperature T. Suppose the potential energy of the system $\phi(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)$ can be expressed as the sum of pairwise intermolecular potential $u(r_{ij})$, $\phi=\Sigma_{1<i<j}^{N}u(r_{ij})$, where $\mathbf{r}_i$ is the position of the ith molecule and $r_{ij}=|\mathbf{r}_i-\mathbf{r}_j|$. In order to study the thermodynamic properties of the system, it is essential to know the radial distribution function $g(r_{12})$, defined by

$$g(r_{12})=V^2\int \bar{e}^{\beta\phi}\,d\mathbf{r}_3\cdots d\mathbf{r}_N\left\{\int \bar{e}^{\beta\phi}\,d\mathbf{r}_1\,d\mathbf{r}_2\cdots d\mathbf{r}_N\right\}^{-1}, \tag{1}$$

where $\beta=1/kT$, and k is the Boltzmann constant.

Since $g(r_{12})\to 1$ as $r_{12}\to\infty$, we define the total correlation function $h(r_{12})$ between molecules 1 and 2 by $h(r_{12})=g(r_{12})-1$. Following Ornstein and Zernike,[1] the total correlation function $h(r_{12})$ can be written as the sum of the direct correlation function $c(r_{12})$ and an indirect correlation function, which accounts for the correlation of molecules 1 and 2 through a third molecule:

$$h(r_{12})=c(r_{12})+\rho\int h(r_{13})c(r_{23})d\mathbf{r}_3. \tag{2}$$

The convolution relation (2) is usually referred to as the Ornstein–Zernike (OZ) relation, which can be considered as the definition of $c(r_{12})$.

Several approximate integral equations for $g(r_{12})$ have been proposed in the past. It is generally accepted that the Percus–Yevick (PY) equation[2] is the most successful theory. In particular, the PY equation for the one-dimensional system of hard rods becomes an exact theory.[3]

Let

$$f(r)=\bar{e}^{\beta u(r)}-1,$$

$$y(r)=e^{\beta u(r)}g(r),\quad r=r_{12}.$$

The PY approximation assumes that $c(r)$ vanishes outside the range of the intermolecular potential $u(r)$ via the relation $c(r)=f(r)y(r)$. The PY approximation in conjunction with the OZ relation (2) forms an integral equation for $g(r)$ in terms of $y(r)$,

$$y(r)=1+\rho\int y(r')f(r')\times[\bar{e}^{\beta u(r-r')}y(r-r')-1]d\mathbf{r}'. \tag{3}$$

Equation (3) has been solved analytically for the hard sphere potential by Wertheim,[4] Thiel,[5] and recently by Chen.[6] Wertheim also had considered an attractive potential with a range less than the diameter σ of the hard spheres. However, his results were not conclusive. On the other hand, by expanding $c(r)$ and $y(r)$ in series of the density ρ, Groeneveld[7] proved the existence of a unique solution of Eq. (3), which was analytic in the region $B|\rho|<(4A)^{-1}$, where

$$A=\mathrm{Sup}_{\mathbf{r}_1,\mathbf{r}_2}\{\bar{e}^{\beta u(|\mathbf{r}_1-\mathbf{r}_2|)}\}<\infty,$$

and

$$B=\mathrm{Sup}_{\mathbf{r}_1}\left\{\int[\bar{e}^{\beta u(|\mathbf{r}_1-\mathbf{r}_2|)}-1]d\mathbf{r}_2\right\}<\infty.$$

In 1968, Watts[8] solved the PY equation via Baxter's[9] relations numerically by truncating the Lennard–Jones potential at $r=3.5\sigma$, $r=5\sigma$, and $r=6\sigma$, respectively. It was concluded that the PY equation exhibited a phase transition characterized by the divergence of the isothermal compressibility with a critical density ρ_c close to the value 0.27, whereas the critical temperature was dependent upon the truncation of this potential. Moreover, outside the critical region the PY equation has two solutions, of which the one in the higher-density region was an unphysical solution.

In a previous paper,[10] we have studied the PY equation by a perturbation method, where the attractive potential was

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considered as a perturbation on the repulsive potential. However, the attractive potential was assumed to be of infinite range and decreases to zero faster than r^{-5} as $r\to\infty$. In light of the interesting results of Watts, in this paper we reexamine the PY equation by a perturbation method for the intermolecular potential $u(r)=u_0(r)-\S v(r)$, where $u_0(r)$ denotes the hard sphere potential of diameter 1, and $v(r)\geqslant 0$, the attractive part of the potential, is a $C^{(2)}$ function on $(1,l)$ with $v(1)=v(l)=0$. For convenience, l is taken to be a positive integer, and § denotes the maximum depth of the physical tail potential so that $\mathrm{Max}|v(r)|\leqslant 1$. The perturbation series is constructed by making use of Baxter's relations and the PY approximation $c(r)=f(r)y(r)$. Within the region of the absolute and uniform convergence of the perturbation series, we show that the PY equation has a unique solution $y(r)$ for $r>0$ if $0<\eta<\frac{1}{2}(3-\sqrt{7})=0.175$, or $1<\eta<2.66$, and a divergent solution if $0.175<\eta<1$, or $\eta>2.66$, where $\eta=\pi\rho/6$. The solution y is a continuous function of r for $r>0$, except for a possible finite discontinuity at $r=1$, and is also a continuous function of η. Based on the solution y, the isothermal compressibility is a continuous bounded function of η if $0<\eta<0.175$, which becomes divergent as $\eta\to 0.175$. The critical density $\eta_c=0.175$ (or $\rho_c=0.33$) is independent of the range of the attractive potential. On the other hand, the critical temperature depends explicitly on the range of the attractive potential. Qualitatively speaking, the results we have obtained are in agreement with the numerical solution of Watts based on the Lennard–Jones potential.

II. PERTURBATION SERIES

Suppose $c(r)=0$ for $r\geqslant l$. Baxter[9] has shown that the OZ relation can be transformed into the following relations provided

$$\tilde{h}(w)=\int e^{i\mathbf{w}\cdot\mathbf{r}}|h(r)|d\mathbf{r} \text{ is bounded for real } w=|\mathbf{w}|:$$

$$rc(r)=-Q'(r)+12\eta\int_r^l Q'(t)Q(t-r)dt,\quad 0\leqslant r\leqslant l, \tag{4}$$

$$rh(r)=-Q'(r)+12\eta\int_0^\infty (r-t)h(|r-t|)Q(t)dt,\quad r\geqslant 0 \tag{5}$$

where $Q(r)$ is a continuous function on $[0,l]$ and $Q(l)=0$.

Relations (4) and (5) are usually referred to as Baxter's relations (BR). In terms of the PY approximation $c(r)=f(r)y(r)$, the PY equation can now be defined as Eqs. (4) and (5) with $c(r)=f(r)y(r)$. For the hard sphere potential, Baxter has solved Eqs. (4) and (5) for $c(r)$ and $Q(r)$. The solution of $c(r)$ is identical to the solutions obtained by Wertheim and Thiel. On the other hand, Eq. (5) can be reduced to a third-order retarded linear differential-difference equation, by which the solution of $y(r)$ can be obtained.[6]

Let $u(r)=u_0(r)-\S v(r)$. If the attractive potential is considered as a perturbation on the hard-sphere potential, we can expand $f(r)=\bar{e}^{\beta u_0(r)+\beta\S v(r)}$ in the series of $\beta\S v(r)$:

$$f(r)=\bar{e}^{\beta u_0(r)}-1+\sum_{n=1}^\infty \frac{1}{n!}(\beta\S)^{(n)}[v(r)]^{(n)}\bar{e}^{\beta u_0(r)}$$

$$=f_0(r)+\sum_{n=1}^\infty \frac{1}{n!}(\beta\S)^{(n)}f_n(r), \tag{6}$$

where $f_n(r)=\bar{e}^{\beta u_0(r)}[v(r)]^n$. Since $(\beta\S)^{-1}=KT/\S$ is the reduced temperature, the expansion of $f(r)$ in (6) becomes an inverse temperature expansion. Consequently, we can write the following series expansions in $\beta\S$:

$$Q(r)=Q_0(r)+\sum_{n=1}^\infty \frac{1}{n!}(\beta\S)^n Q_n(r), \tag{7}$$

$$y(r)=y_0(r)+\sum_{n=1}^\infty \frac{1}{n!}(\beta\S)^n y_n(r), \tag{8}$$

$$h(r)=h_0(r)+\sum_{n=1}^\infty \frac{1}{n!}(\beta\S)^n h_n(r), \tag{9}$$

$$c(r)=c_0(r)+\sum_{n=1}^\infty \frac{1}{n!}(\beta\S)^n c_n(r), \tag{10}$$

where $Q_0(r), y_0(r), h_0(r)$, and $c_0(r)$ denote the unperturbed system with hard sphere potential $u_0(r)$, and

$$h_n(r)=\bar{e}^{\beta u_0(r)}\sum_{i=0}^n \binom{n}{i}[v(r)]^i y_{n-i}(r),\quad n\geqslant 1, \tag{11}$$

$$c_n(r)=\bar{e}^{\beta u_0(r)}\sum_{i=0}^n \binom{n}{i}[v(r)]^i y_{n-i}(r)-y_n(r),\quad n\geqslant 1 \tag{12}$$

are obtained by the relation $c(r)=f(r)y(r)$.

By substituting Eqs. (6)–(12) into Eqs. (4) and (5), we can obtain the following equations:

$$rc_0(r)=-Q_0'(r)+12\eta\int_r^1 Q_0'(t)Q_0(t-r)dt,\quad 0\leqslant r\leqslant 1,$$

$$rh_0(r)=-Q_0'(r)+12\eta\int_0^1 (r-t)h_0(|r-t|)Q_0(t)dt,\quad r\geqslant 0, \tag{13}$$

$$c_0(r)=f_0(r)y_0(r),$$

$$Q_n'(r)=A_n(r)-12\eta\int_0^l (r-t)Q_n(t)dt$$

$$-12\eta\int_{r+1}^l Y_0(t-r)Q_n(t)dt,\quad 0\leqslant r<1, \tag{14}$$

$$Q_n'(r)=B_n(r)+12\eta\int_r^{r+1} Q_0(t-r)Q_n'(t)dt,\quad 1<r\leqslant l-1, \tag{15}$$

$$Q_n'(r)=B_n(r)+12\eta\int_r^l Q_0(t-r)Q_n'(t)dt,\quad l-1\leqslant r\leqslant l, \tag{16}$$

$$Y_n(r)=Q_n'(r)-12\eta\sum_{i=1}^{n-1}\binom{n}{i}\int_r^l Q_0(t-r)Q_n'(t)dt$$

$$-12\eta\int_r^l Q_n(t-r)Q_0'(t)dt$$

$$-12\eta\int_r^{r+1} Q_0(t-r)Q_n'(t)dt,\quad 0\leqslant r<1, \tag{17}$$

$$Y_n(r) = D_n(r) + 12\eta \int_1^r Q_0(r-t) Y_n(t) dt, \quad 1 \leqslant r \leqslant 2, \tag{18}$$

$$Y_n(r) = E_n(r) + 12\eta \int_0^1 Q_0(t) Y_n(r-t) dt, \quad r \geqslant 2, \tag{19}$$

where $Y_n(r) = r y_n(r), A_n(r), B_n(r), D_n(r)$, and $E_n(r)$ depend on Q_m and Y_m for $m < n$ so that in the nth-order perturbation, they can be considered as known functions.

Note that Eq. (13) is precisely the PY equation for the hard sphere potential. It is known[9] that

$$Q_0(r) = \frac{1+2\eta}{2(1-\eta)^2} r^2 - \frac{3\eta}{2(1-\eta)^2} r - \frac{1}{2(1-\eta)}, \quad 0 \leqslant r \leqslant 1,$$

and $Y_0(r)$ is a function of class $C^{(2)}$ on $(1,\infty)$ with the asymptotic condition $[Y_0(r) - r] \to 0$ exponentially as $r \to \infty$. For the following discussions it is not necessary to know $Y_0(r)$ explicitly. By Eqs. (14)–(19), we notice the following procedure of solving these set of equations:

Eq. (16)→Eq. (15)→Eq. (14)→Eq. (18)
→Eq. (19)→Eq. (17).

Since we are not interested in the computation of the thermodynamic quantities of the system, it is unnecessary to carry out the explicit analytical solutions of $Q_n(r)$ and $Y_n(r)$. Rather, we are only interested in the qualitative discussions of the uniqueness and the properties of solutions of $Q_n(r)$ and $Y_n(r)$, and, particularly, their implications to the occurrence of phase transition, so that comparison with the numerical solution of Watts can be made.

III. SOLUTIONS OF PERTURBATION SERIES

In this section we consider the solutions of Eqs. (14)–(19) according to the procedure discussed in the previous section.

(i) $$Q_n'(r) = B_n(r) + 12\eta \int_r^{r+1} Q_0(t-r) Q_n'(t) dt, \quad 1 \leqslant r \leqslant l-1, \tag{15}$$

$$Q_n'(r) = B_n(r) + 12\eta \int_r^{l} Q_0(t-r) Q_n'(t) dt, \quad l-1 \leqslant r \leqslant l. \tag{16}$$

First, we note that Eq. (16) is well defined, whereas Eq. (15) depends on the solution of Eq. (16). Second, Q_n', Q_n'', and Q_n''' are continuous at $r = l-1$, so that Q_n is a class $C^{(3)}$ function on $(1,l)$. On the other hand, in the first-order solution, $B_1(r) = -v(r) y_0(r)$. Thus $B_1(l) = Q_1'(l) = 0$. By induction, we can show that $B_n(l) = Q_n'(l) = 0$. But v', v'' are not defined at $r = 1$ nor at $r = l$. Hence B_n', B_n'' may not exist at $r = l$. For this reason, Eq. (16) cannot be converted into a differential equation by setting the boundary condition at $r = l$.

For convenience, denote $\mu = 12\eta$, $\phi(r) = Q_n'(r)$, $S(r) = B_n(r)$, and $K(t-r) = \phi_0(t-r)$. Equations (15) and (16) can be rewritten as

$$\phi(r) = S(r) + \mu \int_r^{r+1} K(t-r)\phi(t) dt, \quad 1 \leqslant r \leqslant l-1, \tag{15'}$$

$$\phi(r) = S(r) + \mu \int_r^{l} K(t-r)\phi(t) dt, \quad l-1 \leqslant r \leqslant l. \tag{16'}$$

Although K is a continuous function in t and r on $[0,1]\times[0,1]$, it also depends on the parameter μ (or η). Thus $|K|$ is not necessarily bounded for all μ. In order to obtain a unique solution ϕ of Eqs. (15) and (16), which is not only continuous in r on $[1,l]$, but also bounded in μ, we shall impose a rather strong restriction on K, which can be shown to be related to the possibility of a phase transition.

Let $C^{(0)}[1,l]$ be the space of continuous functions on $[1,l]$ with a metric function d defined by the supremum norm. If ϕ is any function of $C^{(0)}[1,l]$, we define an operator $\mathscr{L}$ acting on ϕ by

$$(\mathscr{L}\phi)(r) = \begin{cases} S(r) + \mu \int_r^{r+1} K(t-r)\phi(t) dt, & 1 \leqslant r \leqslant l-1, \quad (15') \\ S(r) + \mu \int_r^{l} K(t-r)\phi(t) dt, & l-1 \leqslant r \leqslant l. \quad (16') \end{cases}$$

Since S is continuous on $[1,l]$, it is clear that $\mathscr{L}\phi \in C^{(0)}[1,l]$. Thus $\mathscr{L}$ transforms $C^{(0)}[1,l]$ into itself. Next, let ϕ, $\bar{\phi} \in C^{(0)}[1,l]$. Then

$$|\mathscr{L}\phi - \mathscr{L}\bar{\phi}| \leqslant \left[\int_r^{r+1} |\mu K(t-r)| dt\right] d(\phi,\bar{\phi}), \quad \text{if } 1 \leqslant r \leqslant l-1,$$

and

$$|\mathscr{L}\phi - \mathscr{L}\bar{\phi}| \leqslant \left[\int_r^{l-r} |\mu K(t)| dt\right] d(\phi,\bar{\phi}) \leqslant \left[\int_0^1 |\mu K(t)| dt\right] d(\phi,\bar{\phi}), \quad \text{if } l-1 \leqslant r \leqslant l.$$

Hence $d(\mathscr{L}\phi, \mathscr{L}\bar{\phi}) \leqslant [\int_0^1 |\mu K(t)| dt]\, d(\phi,\bar{\phi})$, and $\mathscr{L}$ becomes a contraction operator if

$$|\mu| \int_0^1 |K(t)| dt < 1. \tag{20}$$

But $C^{(0)}[1,l]$ with the metric d is a complete metric space. Hence, there exists a unique $\phi \in C^{(0)}[1,l]$, which satisfies Eqs. (15) and (16) if condition (20) is valid.

The function ϕ can be constructed in the following manner.

(1) For $l-1 \leqslant r \leqslant l$, Eq. (16) can be solved by iteration method, that is,

$$\phi = \sum_{n=0}^{\infty} \mu^n \Psi_n, \Psi_0 = S(r),$$

and

$$\Psi_n(r) = \int_r^l K_n(t_n - r) S(t_n) dt_n$$

with

$$K_1(t_1 - r) = K(t_1 - r)$$

and

$$K_n(t_n - r) = \int_r^{t_n} K_1(t_n - t_{n-1}) K_{n-1}(t_{n-1} - r) dt_{n-1}.$$

(2) By the solution of ϕ on $[l-1, l]$, we can solve Eq. (15) by backward continuation. Consider $r \in [l-2, l-1]$. Then

$$\phi(r) = S(r) + \mu \int_r^{l-1} K(t-r)\phi(t)dt + \mu \int_{l-1}^{r+1} K(t-r)\phi(t)dt,$$

and, again, ϕ can be obtained by iteration method. This process can be repeated until the interval $[1,2]$ is reached.

Alternatively, Eq. (15) can be transformed into a third-order linear differential-difference equation of the advanced type:

$$Q_n'''(r) - \frac{6\eta}{1-\eta} Q_n''(r) + \frac{18\eta^2}{(1-\eta)^2} Q_n'(r) + \frac{12\eta(1+2\eta)}{(1-\eta)^2} Q_n(r) = B_n''(r) - \frac{6\eta(\eta+2)}{(1-\eta)^2} Q_n'(r+1) + \frac{12\eta(1+2\eta)}{(1-\eta)^2} Q_n(r+1). \tag{21}$$

Equation (21) can also be solved by the method of backward continuation. For example, in the interval $[l-2, l-1]$, the right-hand side (rhs) of (21) is considered as given. By the solution of Eq. (16), we can compute $Q_n(l-1)$, $Q_n'(l-1)$, and $Q_n''(l-1)$. These are the boundary conditions for Eq. (21). It then follows that there exists a unique function Q_n of class $C^{(3)}$ on $(l-2, l-1)$ that satisfies the boundary condition at $r = l-1$. This process can be repeated until the interval $[1,2]$ is reached. The solution obtained in this manner is of class $C^{(3)}$ on $(1, l-1)$ provided condition (20) is valid.

(ii) $$Q_n'(r) = A_n(r) - 12\eta \int_0^l (r-t) Q_n(t)dt - 12\eta \int_{r+1}^l Y_0(t-r) Q_n(t)dt, \quad 0 \leqslant r < 1. \tag{14}$$

Let

$$a = 12\eta \int_0^1 t Q_n(t)dt,$$

$$b = 12\eta \int_1^l t Q_n(t)dt,$$

$$c = -12\eta \int_0^1 Q_n(t)dt,$$

$$d = -12\eta \int_1^l Q_n(t)dt,$$

$$m(r) = -12\eta \int_{r+1}^l Y_0(t-r) Q_n(t)dt, \quad 0 \leqslant r < 1.$$

Equation (14) can be rewritten as

$$Q_n'(r) = [A_n(r) + m(r)] + (a+b)r + (c+d), \tag{14'}$$

where $A_n(r)$, $m(r)$, b, and d are given, and a and c are yet to be determined. If we set up the boundary condition at $r = 1$, we can easily obtain a continuous function $Q_n(r)$ in $[0,1]$ that satisfies the boundary condition $Q_n(1)$ computed from the solution of $Q_n(r)$ in $[1, l-1]$.

To summarize, there exists a unique continuous function $Q_n(r)$ on $[0,l]$, which satisifes Eqs. (14)–(16) provided condition (20) holds.

(iii) $$Y_n(r) = D_n(r) + 12\eta \int_1^r Q_0(r-t) Y_n(t)dt, \quad 1 \leqslant r \leqslant 2. \tag{18}$$

Since Q_n is of class $C^{(3)}$ on $(1, l-1]$, D_n is also of class $C^{(3)}$ on $(1, l-1]$. Equation (18) can be transformed into a third-order linear differential equation

$$Y_n'''(r) + \frac{6\eta}{1-\eta} Y_n''(r) + \frac{18\eta^2}{(1-\eta)^2} Y_n'(r) - \frac{12\eta(1+2)}{(1-\eta)^2} Y_n(r) = D_n'''(r), \tag{18'}$$

with boundary conditions

$$Y_n(2) = D_n(2) + 12\eta \int_1^2 Q_0(2-t) Y_n(t)dt,$$

$$Y_n'(2) = D_n'(2) - \frac{6\eta}{1-\eta} Y_n(2) + 12\eta \int_1^2 Q_0'(2-t) Y_n(t)dt, \tag{22}$$

$$Y_n''(2) = D_n''(2) - \frac{6\eta}{1-\eta} Y_n'(2) - \frac{18\eta^2}{(1-\eta)^2} Y_n(2) + \frac{12\eta(1+2\eta)}{(1-\eta)^2} \int_1^2 Y_n(t)dt.$$

Now that Eq. (18') is a third-order linear inhomogeneous differential equation, the general solution can be obtained easily. By the boundary condition (22) we can then obtain a unique Y_n of class $C^{(3)}$ on $(1,2]$.

(iv) $$Y_n(r) = E_n(r) + 12\eta \int_{r-1}^r Q_0(r-t) Y_n(t)dt = E_n(r) + 12\eta \int_0^1 Y_n(r-t) Q_0(t)dt, \quad r > 2. \tag{19}$$

It can be checked that $D_n(2) = E_n(2)$. However, since Q_n is at most of class $C^{(1)}$ on $[l-1, l]$, Eq. (19) cannot be converted into a differential difference equation.

In the first-order solution,

$$E_1(r) = -v(r) y_0(r) - Q_1'(r) + 12\eta \int_0^l dt (r-t) h_0(|r-t|) Q_0(t).$$

Thus $E_1(r) \to 0$ exponentially as $r \to \infty$. By Eq. (19) we can obtain the inequality

$$\left[1-12\eta\int_0^1|Q_0(t)dt\right]\sup_{r\in[2,\infty)}|Y_1(r)|\leqslant\sup_{r\in[2,\infty)}|E_1(r)|<\infty$$

and

$$\begin{aligned}Y_1(r+\Delta)-Y_1(r)&=12\eta\left\{\int_{r-1}^{r-1+\Delta}Q_0(r+\Delta-t)Y_1(t)dt\right.\\&\quad\left.+\int_r^{r+\Delta}Q_0(r+\Delta-t)Y_1(t)dt\right\}\\&\to 0 \text{ as } \Delta\to 0.\end{aligned}$$

Hence, Y_1 is continuous for $r\geqslant 2$ and $Y_1(r)\to 0$ as $r\to\infty$.

Let

$$\tilde{Y}_1(s)=\int_2^\infty Y_1(r)e^{-sr}dr,$$

$$\tilde{E}_1(s)=\int_2^\infty E_1(r)e^{-sr}dr,$$

$$\tilde{G}_1(s)=\tilde{F}_1(s)+12\eta\int_0^1\left[\int_{2-t}^2 Y_1(u)e^{-su}du\right]\times Q_0(t)e^{-st}dt,$$

$$\tilde{H}_1(s)=1-12\eta\int_0^1 Q_0(t)e^{-st}dt=s^{-3}e^{-s}[R(s)e^s+L(s)]=s^{-3}e^{-s}H(s),$$

$$G(s)=s^3e^sG_1(s),$$

where

$$R(s)=s^3+\frac{6\eta}{1-\eta}s^2+\frac{18\eta^2}{(1-\eta)^2}s-\frac{12\eta(1+2\eta)}{(1-\eta)^2},$$

$$L(s)=12\eta(1-\eta)^{-2}[(1+2\eta)+(1+\tfrac{1}{2}\eta)s].$$

The Laplace transform of Eq. (19) yields

$$\tilde{Y}_1(s)=\tilde{G}(s)[\tilde{H}(s)]^{-1}. \tag{23}$$

Except for the triple roots at the origin, it can be shown that all roots of $\tilde{H}(s)$ lie in the left-hand side of the complex s plane.[6] We can arrange the roots in order of nondecreasing absolute value with roots of equal absolute value set in any prescribed order. Let $\{s_n\}$ be a sequence of roots arranged in this manner. The inverse Laplace transform of (23) yields

$$Y_1(r)=\sum_{m=1}^{\infty}P_{m-1}(r)e^{s_mr}, \tag{24}$$

where $P_{m-1}(r)e^{s_mr}$ denotes the residue of $e^{sr}\tilde{G}(s)[\tilde{H}(s)]^{-1}$ at a zero s_n of $\tilde{H}(s)$, and $P_{m-1}(r)$ is a polynomial with a degree of $m-1$ at most if s_m is an m-multiple root. By Theorems 6.5 and 6.6 of Bellman–Cooke,[11] the series expansion in Eq. (24) is convergent for $r\geqslant 2$ and uniformly convergent over any finite interval for $r\geqslant 2$. Since Y_1 is continuous and $Y_1\to 0$ as $r\to\infty$, the residue at $s=0$ must be zero. Thus, by Eq. (24), $Y_1\to 0$ exponentially as $r\to\infty$.

The solution described for $Y_1(r)$ can be generalized for all orders of perturbation. By induction, we can conclude that Eq. (19) has a unique solution for $r\geqslant 2$, which can be expressed as a uniformly convergent generalized Fourier series type of expansion as given in Eq. (24) over any finite interval for $r\geqslant 2$. Furthermore, $Y_n(r)\to 0$ exponentially as $r\to\infty$.

It is interesting to note that Eqs. (15), (16), and (19) are special cases of

$$Y(r)=D(r)+\mu\int_{\alpha(r)}^{\beta(r)}K(t,r)Y(t)dt,\quad r\geqslant 0, \tag{25}$$

where D,α,β are continuous on $I_1=[0,\infty)$, $0\leqslant\alpha(r)<\beta(r)$, and K is continuous on $R=I_1\times I_2$ with $I_2=[\inf\alpha(r),\ \sup\beta(r)]$.

Let $C^{(0)}(I_1)$ be endowed with the metric d defined by the supremum norm. If $Y,\bar{Y}\in C^{(0)}(I_1)$, then

$$d(LY,L\bar{Y})\leqslant d(Y,\bar{Y})\left[|\mu|\sup_{r\in I_1}\int_{\alpha(r)}^{\beta(r)}|K(t,r)|dt\right],$$

where L is an operator which transforms Y into

$$LY=D+\mu\int_{\alpha(r)}^{\beta(r)}K(t,r)Y(t)dt\in C^{(0)}(I_1).$$

Thus, Eq. (25) has a unique solution Y in $C^{(0)}(I_1)$ if

$$|\mu|\sup_{r\in I_1}\int_{\alpha(r)}^{\beta(r)}|K(t,r)|dt<1. \tag{26}$$

This solution can be expressed as an absolutely and uniformly convergent series $Y(r)=\sum_{n=0}^{\infty}\mu^n\Psi_n(r)$, where

$$\Psi_0(r)=D(r),$$

$$\Psi_n(r)=\int_{\alpha(r)}^{\beta(r)}K(t,r)\Psi_{n-1}(t)dt,\quad n\geqslant 1.$$

If we set $\alpha(r)=r-1$, $\beta(r)=r$, and $K(t,r)=Q_0(r-t)$, then condition (26) becomes condition (20).

(v)
$$\begin{aligned}Y_n(r)=Q_n'(r)&-12\eta\sum_{i=1}^{n-1}\binom{n}{i}\times\int_r^l Q_0(t-r)Q_n'(t)dt\\&-12\eta\int_r^1 Q_n(t-r)Q_0'(t)dt\\&-12\eta\int_r^{r+1}Q_0(t-r)Q_n'(t)dt,\quad 0\leqslant r<1.\end{aligned} \tag{17}$$

By the solutions of Eqs. (15) and (16), Y_n can easily be obtained by Eq. (17). However, Y_n may have a finite discontinuity at $r=1$.

Based on the solutions of Eqs. (14)–(19), we can conclude that, to every order of β §, the PY equation has a unique solution $Y_n(r,\eta)$ and a unique solution $Q_n(r,\eta)$ if $12\eta\int_0^1|K(t)|dt<1$. As a function of r, $Q_n\in C^{(0)}[1,l]$ and $Y_n\in C^{(0)}[0,\infty)$ except for a possible finite discontinuity at $r=1$. Furthermore, $Y_n\to 0$ exponentially as $r\to\infty$. On the other hand, by Q_0, both Q_n and Y_n are also continuous functions of η within the region specified by condition (20).

IV. CONVERGENCE OF PERTURBATION SERIES AND PHASE TRANSITION

We now examine condition (20) in detail. According to the expression of Q_0, condition (20) implies $0<\eta<\frac{1}{2}(3-\sqrt{7})=0.175$, or $1<\eta<2.66$. Thus, in terms of the parameter η, the PY equation has two disjoint branches of solutions, one in the region $0<\eta<0.175$, and the other in the region $1<\eta<2.66$. The solution for $\eta>1$ must be con-

sidered as an unphysical solution because η (or ρ) is too high. As $\eta \to \eta_0 = 0.175$, $12\eta\int_0^1 |K(t)|dt \to 1$, and the sequence obtained by successive iterations will no longer form a Cauchy sequence. Thus Q_n and Y_n become divergent. If $\eta > 0.175$, then $12\eta\int_0^1 |K(t)|dt > 1$, and the operators $\mathscr{L}$ or L defined in Eqs. (15) and (16) or Eq. (25) are not contraction operators. In this case, uniqueness of the solutions for Eqs. (15) and (16) or Eq. (25) cannot be guaranteed. For example, suppose v is at least twice-differentiable, and v is also flat enough near $r = l$ so that $v(l) = v'(l) = v''(l) = 0$. In this case Eq. (16) also can be transformed into a third-order linear differential equation, and Eq. (15) can be solved via a differential-difference equation of advanced type for $r \in [1, l-1]$ with the solution of Eq. (16) as initial condition for $r \in [l-1, l]$. But Eqs. (15) and (16) depend on η. It is impossible to examine the η dependence of Q_n unless explicit solutions can be obtained. For this reason, condition (20) is absolutely necessary.

Suppose $0 < \eta < 0.175$. Then $\mathrm{Sup}_{r\in[0,l]}|Q_n|$ and $\mathrm{Sup}_{r>0}|Y_n|$ are continuous and bounded functions of η. So far we have not been able to estimate the upper bound of Q_n and Y_n. But, for any fixed $\eta \in (0, 0.175)$, if $\mathrm{Sup}|Q_n| < n!$ and $\mathrm{Sup}|Y_n| < n!$, then the perturbation series for Q and Y are absolutely and uniformly convergent for $0 < \beta\S < (\beta\S)_0$, where $(\beta\S)_0$ is the radius of convergence of $\beta\S$ which may be greater than 1. To summarize, suppose the following conditions are satisfied:

(i) $0 < \eta < 0.175$,

(ii) $0 < \beta\S < (\beta\S)_0$,

(iii) $\sup_{r\in[0,l]} |Q_n| < n!$, $\sup_{r<0} |Y_n| < n!$.

Then the PY equation has a unique solution $Q(r, \eta, \beta\S)$ and a unique solution $Y(r, \eta, \beta\S)$, where Q is continuous in $\eta, \beta\S$, and, as a function of r, $Q \in C^{(0)}[0,l]$. Similarly, Y is continuous in $\eta, \beta\S$, and as a function of r, Y is continuous except for a finite discontinuity at $r = 1$. Furthermore, $Y - r \to 0$ exponentially as $r \to \infty$.

Since no explicit solutions for Q nor Y have been obtained, it is almost impossible to study the critical region in terms of the critical exponents so that comparison with other well known results can be made.[12] However, based on our qualitative discussions of Q and Y, some interesting conclusions can be obtained as follows.

(1) The isothermal compressibility equation can be written as[13]

$$kT\left(\frac{\partial\rho}{\partial p}\right)_T = K_T = 1 + 24\eta\int_0^\infty r^2[g(r) - 1]dr, \tag{27}$$

which can be rewritten as[9]

$$\frac{1}{kT}\left(\frac{\partial P}{\partial\rho}\right)_T = 1 - 24\eta\int_0^l r^2 c(r)dr = \left[1 - 12\eta\int_0^l Q(r)dr\right]^2, \tag{28}$$

where P is the pressure. By definition, $g(r) = 0$ for $r < 1$, and $g(r) = e^{\beta\S v(r)}y(r)$ for $r > 1$. Thus, by the absolute and uniform convergence of Q and Y, K_T is a continuous bounded function of $\eta \in (0, 0.175)$. As $\eta \to 0.175$, $K_T \to \infty$, and, as $\eta > 0.175$, K_T is no longer a unique function of η. From a physical point of view, it is essential that K_T is a unique, continuous, bounded function of η outside the critical region. In this sense, $\eta_c = 0.175$ can be identified as the critical density. It is interesting to note that $\eta_c = 0.175$ corresponds to $\rho_c = 0.33$, which is close to the critical density $\rho_c = 0.27$, obtained by Watts for the Lennard–Jones potential. Moreover, the value of η_c is independent of the range of the attractive potential. On the other hand, by Eq. (28), the critical temperature $(\beta\S)_c$ is determined by the condition $F(\beta\S) = 1$, where $F(\beta\S) = 12\eta\int_0^l Q(r)dr = 0$. It is evident that $(\beta\S)_c$ depends explicitly on the range of the attractive potential.

(2) Since $Y_n \to 0$ exponentially as $r \to \infty$, by Eq. (24), the closest root s_1 of $H(s)$ to the origin in the left half-plane therefore determines the asymptotic behavior of Y_n. For $r \gg l$, we have $h(r) \sim R(\beta\S, \eta)e^{s_1 r}/r$, where $R(\beta\S, \eta)$, denotes the residue at s_1. Thus $h(r)$ decays exponentially for large r. However, s_1 is a function of η, which does not vanish at $\eta_c = 0.175$. Hence, $h(r)$ does not have the long-range behavior of $1/r$ in the critical region.[12] The divergence of the isothermal compressibility at the critical point is due to the divergence of $g(r)$ rather than the long-range asymptotic behavior of $1/r$.

(3) The energy equation can be written as[13]

$$U = \frac{3}{2}N\beta^{-1} + 12\eta N\int_1^l r^2 v(r)g(r)dr,$$

which is related to the Helmholtz free energy A by

$$U = \left[\frac{\partial(A/T)}{\partial(1/T)}\right]_V.$$

At very high temperatures, $v(r)$ is negligible compared to kT, and thus the intermolecular potential $u(r)$ becomes the hard sphere potential. Hence, the free energy A can be obtained by integrating the energy equation:

$$\frac{A}{NkT} = \int_0^{\beta\S}\frac{1}{\beta\S}Ud(\beta\S)' = \frac{A_0}{NkT} + 12\eta\int_0^{\beta\S} d(\beta\S)'\int_1^l r^2 v(r)g(r), \tag{29}$$

where A_0 is the free energy of the hard sphere potential. Since $g(r)$ can be expanded in series of $\beta\S$, we can write $A = A_0 + \beta\S A_1 + \beta\S A_2 + \cdots$. To the first order we have

$$\frac{A}{NkT} = \frac{A_0}{NkT} + 12\eta\beta\S\int_1^l r^2 v(r)g_0(r)dr. \tag{30}$$

For the square-well potential, we have computed A_1 and A_2 (see Ref. 14). Compared with the Monte Carlo calculations, the result for A_1 was excellent. The result for A_2 was very good at low densities. However, at high densities, it appeared to be too small in absolute magnitude. It is interesting to note that Eq. (30) also can be obtained by considering the stationary solution of a kinetic equation of the Enskog–Vlasov type studied by de Sobrino[15] and by Grmela.[16] By Eq. (30) we can obtain an equation of state similar to the van der Waals equation of state. For the PY theory, $g_0(r)$ can be expressed in terms of elementary functions with extremely complicated coefficients in η. It is thus impossible to study Eq. (30) analytically.

To conclude, from a qualitative point of view, our results seem to be in agreement with the numerical solution of Watts. We have also identified the critical point with the following possibilities: (i) $g(r)$ is divergent so that the isothermal compressibility K_T is also divergent; and (ii) $g(r)$ may have multiple solutions, among them one is divergent. Thus, there is no unique K_T at the critical point. The second possibility is closely related to the Kirkwood–Monroe[17] theory of phase transition, which is defined as a discontinuity in $g(r)$ when the thermodynamic parameters η and β § are varied.

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An alternate proof of ultraviolet stability of the two-dimensional massive sine–Gordon field theory in all regions of collapse

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The upper bound for the ultraviolet stability of the two-dimensional cosine interaction $\int_\Lambda :\cos \alpha\varphi_\xi: d\xi$, $\Lambda \subset \mathbb{R}^2$, in finite volume Λ is proven for $\alpha^2 \in [4\pi, 8\pi[$, where the theory has been shown to be superrenormalizable [see, e.g., G. Gallavotti, Rev. Mod. Phys. **57**, 471 (1985)]. Ultraviolet stability in this interval was proven previously (F. Nicolò, J. Renn, and A.Steinmann, "On the massive sine–Gordon equation in all regions of collapse," preprint II Università di Roma, 1985). Here we give a second proof using renormalization group methods based on a multiscale decomposition of the field by showing that the large fluctuations may be controlled by their small probability. The method essentially follows the one given by Nicolò [F. Nicolò, Commun. Math. Phys. **88**, 681 (1983)] for $\alpha^2 \in [4\pi, \frac{32}{5}\pi[$.

I. INTRODUCTION

A. Purpose and outline

The two-dimensional sine–Gordon model has been studied as a problem in constructive quantum field theory in a series of articles,[1–4] which finally led to the proof of its ultraviolet stability for all α^2 in the interval $[0,8\pi[$, i.e., for the whole range of α^2 for which the model is superrenormalizable as a field theory.[1] (For $\alpha^2 \in [0,4\pi[$, only Wick ordering is required in order to have a finite theory.) The proof in Ref. 1 was based on renormalization group methods and on an extensive use of the tree formalism, both introduced in Refs. 5 and 6. The difficult problem to solve, however, was the treatment of the large fluctuations of the random fields arising in the Euclidean formalism. The solution given in Ref. 1 exploited certain negativity properties of these large fluctuation parts in a more systematic way than was done in previous work (cf. Refs. 2 and 3). Here we give a second proof of ultraviolet stability in the interval $[4\pi,8\pi[$, for which probability estimates of the large fluctuations play the more important role. This second solution generalizes the methods used for values $[4\pi, \frac{32}{5}\pi[$ in Ref. 2 [we only prove the upper bound of ultraviolet stability (cf. Ref. 3) since for the proof of the lower bound the large fluctuating fields present no problem]. Contrary to the first approach to the problem of stability for $\alpha^2 \geqslant 4\pi$ in Ref. 3 the solution given in Ref. 1 as well as the one presented here also rely on an iterative procedure for treating the large fluctuation parts of the fields in the spirit of the renormalization group. Since the formalism and the notation used are explained in complete detail in Ref. 1 we will restrict ourselves here to a brief summary. Furthermore, we will make extensive use of the estimates of the effective potentials associated to different scales derived in Ref. 1.

B. The Pauli–Villar regularization, the renormalized interaction, and the ultraviolet stability of the sine–Gordon theory

Let the multiscale decomposition

$$\varphi_\xi^{(<N)} = \sum_{h=0}^{N} \varphi_\xi^{(h)} \tag{1.1}$$

denote a regularized free field with ultraviolet cutoff γ^{-N}, where $\gamma > 1$ is a scaling parameter chosen close to 1 and the covariances of the regular fields $\varphi_\xi^{(h)}$ on scale h are given by a Pauli–Villar regularization of first order:

$$C^{(h)}(\xi-\eta) := C_{\xi\eta}^{(h)} := \int dp\, e^{ip(\xi-\eta)} \times \left(\frac{1}{p^2+\gamma^{2h}} - \frac{1}{p^2+\gamma^{2h+2}}\right). \tag{1.2}$$

The "bare cosine interaction with cutoff N"

$$V_0^{(N)}[\Lambda] := V_0(\varphi^{(<N)})[\Lambda] := \frac{\lambda}{2}\int_\Lambda \sum_{\sigma=\pm 1} :e^{i\alpha\sigma\varphi^{(<N)}}\xi: d\xi \tag{1.3}$$

is superrenormalizable for all values $\alpha^2 \in [4\pi,8\pi[$, where the field theory is meaningful and has a Yukawa gas interpretation in statistical mechanics.[1–3] (Note that the Wick ordering is defined by: $e^{f}:\equiv e^{-(1/2)\mathscr{E}(f^2)} e^{f}$.)

Let $\mathscr{E}_h(\cdot)$ denote the expectation with respect to the Gaussian measure $P(d\varphi^{(h)})$ given by the covariance $C_{\xi\eta}^{(h)}$ in (1.2). For n random variables $f_1,\ldots,f_n$ we define the "truncated expectation" or "cumulant" of order n with respect to a Gaussian measure as follows:

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$$\mathscr{E}^T(f_1,\dots,f_n) := \frac{\partial^n}{\partial\tau_1\cdots\partial\tau_n}\log\mathscr{E}(e^{\tau_1 f_1+\cdots+\tau_n f_n})\Big|_{\tau_1=\cdots=\tau_n=0}. \tag{1.4}$$

Further, we write $\mathscr{E}^T(f;n)$ when $f_1=\cdots=f_n=f$. Note that the cumulants are multilinear and $\mathscr{E}^T(\cdot;1)=\mathscr{E}(\cdot)$. Finally, we write $\mathscr{E}_{(<k)}$ for the product $\mathscr{E}_0\cdots\mathscr{E}_k$; i.e., the expectation with respect to the product measure ($\forall k\in\mathbb{N}$):

$$P(d\varphi^{(<k)}) = \prod_{h=0}^{k} P(d\varphi^{(h)}). \tag{1.5}$$

Using this notation we introduce the "renormalized cosine interaction up to order t" for any even integer t satisfying $t\geqslant t_0$ such that for $t_0\in\mathbb{N}$, $t_0>1$, and

$$\alpha^2\in[8\pi(1-1/t_0),8\pi(1-1/(t_0+2))[, \tag{1.6}$$

$$V^{(N)}[\Lambda] := V(\varphi^{(<N)})[\Lambda] := V_0(\varphi^{(<N)})[\Lambda] - \sum_{n=1}^{t}\frac{1}{n!}\mathscr{E}^T_{(<N)}(V_0^{(N)}[\Lambda];n). \tag{1.7}$$

The counterterms (i.e., the cumulants) are constants that may be infinite as the cutoff is removed (i.e., $N\to\infty$); note, however, that odd-order counterterms remain finite by the nature of the bounds of the effective potential on the scale k (cf. Ref. 1, Theorem 2.1). The $V^{(N)}[\Lambda]$ is called "stable in the ultraviolet limit" if there exist two positive constants $E_-(\lambda)$ and $E_+(\lambda)$ independent of the cutoff N and of the finite volume Λ so that

$$e^{-E_-(\lambda)|\Lambda|}\leqslant\int e^{V^{(N)}[\Lambda]}P(d\varphi^{(<N)})\leqslant e^{+E_+(\lambda)|\Lambda|}. \tag{1.8}$$

Moreover, we will show that in our case the constants $E_\pm(\lambda)$ satisfy the following property:

$$\lim_{\lambda\to0}E_\pm(\lambda)\lambda^{-(t+\tau)}=0, \tag{1.9}$$

for some $\tau>0$.

C. The effective potential

It will be convenient to study the effective interaction on the scale k defined recursively for $k=0,\dots,N-1$,

$$V^{(k)}[\Lambda] := V^{(k)}(\varphi^{(<k)})[\Lambda] := \log\mathscr{E}_{k+1}(e^{V^{(k+1)}}[\Lambda]), \tag{1.10}$$

as we perform the successive functional integrations with respect to the measures $P(d\varphi^{(h)})$ for $h=N,N-1,\dots,k+1$. By expanding the right-hand side of (1.10) into a formal Taylor series one gets

$$V^{(k)}[\Lambda] = \sum_{n=0}^{\infty}\frac{1}{n!}\mathscr{E}^T_{k+1}(V^{(k+1)}[\Lambda];n). \tag{1.11}$$

By iterating this procedure for the effective potential in the arguments of the rhs of (1.11), the Gallavotti–Nicolò tree expansion may be derived.[5,6] Generally we will be interested only in the contributions to $V^{(k)}[\Lambda]$ up to a certain order t in λ; that is we study the "truncated effective potential" on the scale k:

$$\tilde{V}^{(k)}[\Lambda] := \tilde{V}^{(k)}(\varphi^{(<k)})[\Lambda] := [V^{(k)}[\Lambda]]_{<t}, \tag{1.12}$$

where $[\cdot]_{<t}$ means that we drop orders in λ higher than t.

II. THE PREREQUISITES TO THE PROOF

A. The recursive procedure

The recursive procedure that we are going to construct will make use of the fact that the integration with respect to the measure $P(d\varphi^{(<N)})$ can be factorized into a sequence of integrations with respect to the measures $P(d\varphi^{(k)})$ ($k=0,\dots,N$) due to the multiscale decomposition of the field. In fact, we will have to study explicitly only a single one of these integrations due to the scale invariance

$$\varphi^{(h)}_\xi = \varphi^{(0)}_{\gamma^h\xi}\quad(\forall h\in\mathbb{N}) \tag{2.1}$$

of the regular Gaussian fields $\varphi^{(h)}_\xi$. Proceeding heuristically for now, let us restrict ourselves to "smooth fields," i.e., fields in the set ($0<\epsilon\ll1$, to be chosen later):

$$\{\varphi^{(k)}\,|\,|\sin((\alpha/2)(\varphi^{(k)}_\xi-\varphi^{(k)}_\eta))| \leqslant B_k(\gamma^k|\xi-\eta|)^{1-\epsilon},\quad\forall\xi,\eta\in\Lambda\}, \tag{2.2}$$

whose characteristic function we call χ^{B_k} given the increasing succession[5] $\{B_k\}$

$$B_k := B(1+k)^{\tilde{a}}\log(e+k+\lambda^{-1}), \tag{2.3}$$

with $\tilde{a}\geqslant2$ and $B>1$ arbitrarily fixed.

After having integrated $\exp(\tilde{V}^{(N)}[\Lambda])$ with respect to these smooth fields from scale N down to scale k, we can expect to find $\chi^{B_k}\exp(\tilde{V}^{(k)}[\Lambda])$ multiplied by a remainder of higher order, i.e., an expression like

$$\chi^{B_k}\exp\{\tilde{V}^{(k)}[\Lambda]+\lambda^{t+1}R(t,\lambda,\varphi^{(<k)})\},$$

where $R(t,\lambda,\varphi^{(<k)})$ is a remainder, which, of course, depends on λ, on the truncation order t, and on the fields with respect to which we have not integrated yet. That these integrations can indeed be performed with $R(t,\lambda,\varphi^{(<k)})$ a remainder of controllable size, is guaranteed by the so-called "Main Lemma," which we will state in complete detail in Sec. II B. The necessary prerequisite for applying the Main Lemma to the integration with respect to the Gaussian measure $P(d\varphi^{(k)})$ are good estimates on the smooth part of the effective potential $\tilde{V}^{(k)}[\Lambda]$. Such estimates have, in fact, been derived in Ref. 1. The recursive procedure comes to an end at some finite frequency k_0 for which it will be an easy task to prove inequality (1.8), provided the recursive procedure has produced sufficiently strong estimates on the smooth part of the effective potential and on the remainder at the finite frequency k_0.

The iterative procedure we have described thus far only applies to the smooth part of the effective potential (i.e., the part depending on the smooth fields), because the estimates of the effective potential that we have mentioned are only valid for this part. In principle, there are two ways of treating

the large fluctuation contributions to the effective potential in the proof of the upper bound of ultraviolet stability: either they can be neglected because they are negative or they have to be considered as additional contributions to the remainders $R(t,\lambda,\varphi^{(<k)})$. In the proof given in Ref. 1 as well as in the one presented here, both of these treatments are used, although the emphasis in Ref. 1 is on negativity properties whereas here it is on careful probability estimates of the large fluctuation contributions.

It turns out that it is not possible to cope with the problem of large fluctuations considering only a single scale. In fact, just as the smooth part of $\tilde{V}^{(k_0)}[\Lambda]$ has to be considered—in agreement with the philosophy of the renormalization group—as produced by contributions coming from different scales k ($k_0 \leqslant k \leqslant N$), which are to be treated step by step, also the large fluctuation part of $\tilde{V}^{(k_0)}[\Lambda]$ has to be accurately decomposed into components originating on different scales. Having recognized this general fact it is of secondary importance whether the decomposition of the large fluctuation part is done to exhibit further negativity properties (cf. the proof in Ref. 1) or to distribute estimates of the large fluctuations over the remainders appearing at different scales. In this paper we will, in fact, follow the latter strategy.

Before doing so, however, we should make more precise the notions "smooth" and "large fluctuation part" of the effective potential at frequency k, but without rewriting here the complicated definitions given in Ref. 1. Thus, we only briefly present the main ingredients of the iterative mechanism used, referring the reader to Ref. 1 for their precise definitions (cf. Sec. 2 of Ref. 1). The different parts of the effective potential at frequency k we have to consider are distinguished according to the regions in $\mathbb{R}^{2t}$ over which they are integrated (in the same sense as $V_0^{(N)}[\Lambda]$ is integrated over $\Lambda \subset \mathbb{R}^2$). These regions of integration in turn are characterized by the behavior of the fields $\varphi^{(k)}$, $\varphi^{(<k)}$, and $\varphi^{(<k-1)}$. Let us, for now heuristically, indicate the regions of integration in which the field $\varphi^{(k)}$ has large fluctuations by $\mathscr{R}_k$ and those in which the fields $\varphi^{(<k)}$ or $\varphi^{(<k-1)}$ have large fluctuations by $\mathscr{D}_k$ (resp. $\mathscr{D}_{k-1}$) (and their complements by $\mathscr{R}_k^c, \mathscr{D}_k^c, \mathscr{D}_{k-1}^c$). The precise definitions are given in Sec. III A. Due to the relationship between large fluctuations of different frequencies (a large fluctuation of $\varphi^{(<k)}$ is either caused by a large fluctuation of $\varphi^{(k)}$ or of $\varphi^{(<k-1)}$) we have the following inclusion (cf. Lemma 3.1; the regions considered here are, however, more complicated than those of Lemma 3.1, nevertheless a similar inclusion holds, as is shown in Sec. 2 of Ref. 2):

$$\mathscr{D}_k \subset \mathscr{D}_{k-1} \cup \mathscr{R}_k. \tag{2.4}$$

This relationship is used to simplify the integration of the smooth part of the effective potential $\tilde{V}^{(k)}[\Lambda]$ with respect to $P(d\varphi^{(k)})$. Although it would be natural to consider $\tilde{V}^{(k)}[\mathscr{D}_k^c]$ as the smooth part of $\tilde{V}^{(k)}[\Lambda]$, the dependence on the field $\varphi^{(<k)}$ introduced by the region of integration $\mathscr{D}_k^c$ of $\tilde{V}^{(k)}[\mathscr{D}_k^c]$ is very hard to control. Therefore, one uses (2.4), which allows one to consider $\tilde{V}^{(k)}[\mathscr{D}_{k-1}^c \cap \mathscr{R}_k^c]$ as a smooth part of $\tilde{V}^{(k)}[\Lambda]$, where now, however, the dependence on $\varphi^{(k)}$ introduced by $\mathscr{R}_k^c$ turns out to be manageable. When integrating this expression with respect to $P(d\varphi^{(k)})$ by using the Main Lemma one obtains an expression of the following type [cf. (1.11)]:

$$\left[\sum_{n=1}^{t} \frac{1}{n!} \mathscr{E}_k^T(\tilde{V}^{(k)}[\mathscr{D}_{k-1}^c];n)\right]_{<t} + \text{controllable remainder.}$$

From the above it is clear that we can construct an iterative procedure for the proof of the upper bound of ultraviolet stability if the following steps can be performed (the integration of $\tilde{V}^{(N)}[\Lambda]$ with respect to $P(d\varphi^{(N)})$ is trivial):

(1) $V^{(N-1)}[\Lambda] \to V^{(N-1)}[\mathscr{D}_{N-1}^c]$,

(2) $\tilde{V}^{(k)}[\mathscr{D}_k^c] \to \tilde{V}^{(k)}[\mathscr{D}_{k-1}^c \cap \mathscr{R}_k^c]$

(3) $\tilde{V}^{(k)}[\mathscr{D}_{k-1}^c \cap \mathscr{R}_k^c] \to \left[\sum_{n=1}^{t} \frac{1}{n!} \mathscr{E}_k^T(\tilde{V}^{(k)}[\mathscr{D}_{k-1}^c];n)\right]_{<t}$,

(4) $\left[\sum_{n=1}^{t} \frac{1}{n!} \mathscr{E}_k^T(\tilde{V}^{(k)}[\mathscr{D}_{k-1}^c];n)\right]_{<t} \to \tilde{V}^{(k-1)}[\mathscr{D}_{k-1}^c]$.

It is not difficult to show that steps (1) and (2) are indeed allowed, since

(a) $V^{(N-1)}[\mathscr{D}_{N-1}] \leqslant 0$,

(b) $\tilde{V}^{(k)}[\mathscr{D}_k^c \cap \mathscr{D}_{k-1} \cap \mathscr{R}_k^c] \leqslant 0$,

(c) $\tilde{V}^{(k)}[\mathscr{D}_k^c \cap \mathscr{R}_k]$ gives rise to a controllable remainder.

Here, (a) and (b) are negativity properties of large fluctuation parts of the effective potential, together with (c) they have been shown in Ref. 1 (cf. also Ref. 3).

Step (3) can be performed using the Main Lemma. Step (4) is the fundamental difficulty of the proof that was first encountered in Ref. 3. It is here that it becomes clear that the large fluctuation problem cannot be solved without taking into account more systematically the relationship of large fluctuations of different scales. What one has to do, in fact, is to create a transport mechanism for the large fluctuation part of the effective potential, which is the equivalent of the transport of its smooth part by the Main Lemma.

In Sec. III we will show how the difference

$$\Delta^{(k-1)}[\mathscr{D}_{k-1}] := \left[\sum_{n=1}^{t} \frac{1}{n!} \mathscr{E}_k^T(\tilde{V}^{(k)}[\mathscr{D}_{k-1}^c];n)\right]_{<t} - \tilde{V}^{(k-1)}[\mathscr{D}_{k-1}^c] \tag{2.5}$$

can be decomposed into components coming from different scales. But before doing so let us state the Main Lemma.

B. The Main Lemma

Consider a function $H(J)$ of the fields $\varphi^{(k)}$ at fixed fields $\varphi^{(<k-1)}$ given an arbitrary set $J \subset \Lambda$ [$\underline{p} = (p_1,\ldots,p_m)$, $\underline{q},\underline{m}$ analogously; $p_i,q_i,m_i \geqslant 0$]

$$H[J](\varphi^{(k)}) := H^{(k)}[J] := \sum_{n=1}^{t}\sum_{m=1}^{n}\sum_{\substack{p_i \\ 0<\sum_{i=1}^{m} q_i < m \\ m_i}} \left\{\lambda^h \int_{J^h} d\xi_1 \cdots d\xi_h\, v_{pqm}(\xi_i,\ldots,\xi_h) \prod_{j=1}^{m}\left(\cos\frac{\alpha}{2}\varphi_{\xi_j}^{(<k)}\right)^{p_j}\right.$$

$$\left.\times \prod_{j=1}^{m}\left[\left(\sin\frac{\alpha}{2}\varphi_{\xi_j}^{(<k)}\right)^{p_j}\sum_{\substack{j'=1 \\ j'\neq j}}^{m}\left(\frac{\sin(\alpha/2)(\varphi_{\xi_j}^{(<k)}-\varphi_{\xi_{j'}}^{(<k)})}{(\gamma^k|\xi_j-\xi_{j'}|)^{1-\epsilon}}\right)^{m_j}\right]\right\}, \tag{2.6}$$

where $0<\epsilon<\frac{1}{2}$ and $\gamma>1$ are arbitrarily fixed parameters of Hölder continuity and scaling.

Assuming Q_k to be an exact pavement of Λ, i.e., $\cup_{\Delta\in Q_k}\Delta=\Lambda$, where the Δ are squares of side length γ^{-k}. Let $d(\Delta_1,\ldots,\Delta_n)$ be the length of the shortest path connecting $\Delta_1,\ldots,\Delta_n$. The kernels V_{pqm} of $H[J]$ are supposed to satisfy bounds of the following type:

$$\lambda^n\int_{\Delta_1\times\cdots\times\Delta_n}|v_{pqm}(\xi_1,\ldots,\xi_n)|d\xi_1\cdots d\xi_n$$

$$\leqslant(\text{const})e^{-\kappa\gamma^k d(\Delta_1,\ldots,\Delta_n)}B_k^2\lambda_{\text{eff}}^n(k)$$

$$\leqslant\overline{H}_k e^{-\kappa\gamma^k d(\Delta_1,\ldots,\Delta_n)}, \tag{2.7}$$

where $\lambda_{\text{eff}}(k)$ is the effective coupling constant defined by

$$\lambda_{\text{eff}}(k) := \lambda\gamma^{(\alpha^2/4\pi-2)k}, \tag{2.8}$$

B_k is the increasing succession given by (2.3), and (for large k on small λ) $\overline{H}_k$ may be chosen independent of n as $\overline{H}\lambda_{\text{eff}}(k)B_k^2$; $\overline{H}$ and κ are positive constants.

We further define the $P(d\varphi^{(k)})$-measurable events

$$E_\Delta^B := \left\{\varphi^{(k)}\,|\sup_{\xi,\eta\in\Delta}\left[\frac{|\varphi_\xi^{(k)}-\varphi_\eta^{(k)}|}{(\gamma^{(k)}|\xi-\eta|)^{1-\epsilon}}\right]\right.$$

$$\left.\leqslant B(1+\gamma^{(k)}d(\Delta,J))\right\}, \tag{2.9}$$

whose characteristic functions we call χ_Δ^B. Defining

$$\mathring{\chi}_\Delta^B := 1-\chi_\Delta^B \tag{2.10}$$

and for arbitrary $G\subset J$

$$\chi_{Q_k\setminus G}^B := \prod_{\Delta\in Q_k\setminus G}\chi_\Delta^B,$$
$$\mathring{\chi}_G^B := \prod_{\Delta\in G}\mathring{\chi}_\Delta^B, \tag{2.11}$$

we have the following decomposition of the identity:

$$\sum_{G\subset Q_k}\mathring{\chi}_G^B\,\chi_{Q_k\setminus G}^B\equiv 1. \tag{2.12}$$

Using these definitions the Main Lemma can be stated as follows.

Lemma 2.1 (Main Lemma): For every integer $t>0$ there exist constants B^*, D, g, g' depending only on ϵ, γ, t, and κ so that for $B>B^*$

$$\int\mathring{\chi}_G^B\,\chi_{J\setminus G}^B e^{H[J\setminus G](\varphi^{(k)})}P(d\varphi^{(k)})$$

$$\leqslant\exp\{\delta(B,\overline{H}_k)\gamma^{2k}|J|+\delta'(B,\overline{H}_k)\gamma^{2k}|G\cap J|\}$$

$$\times\exp\left[\sum_{p=1}^{t}\frac{1}{p!}\mathscr{E}_k^T(H[J](\varphi^{(k)});p)\right]_{<t}$$

$$\times\left(\int\mathring{\chi}_G^B P(d\varphi^{(k)})\right)^{1/2}, \tag{2.13}$$

where

$$\delta(B,\overline{H}_k) := D\{(\overline{H}_k B^g e^{g\overline{H}_k B^g})^{t+1}+e^{-g'B^2+g\overline{H}_k B^g}\},$$
$$\delta'(B,\overline{H}_k) := D\{\overline{H}_k B^g\}. \tag{2.14}$$

Further, we have an estimate on the probability that the event E_Δ^B does not occur, i.e., the probability of a large fluctuation: For all $\epsilon>0$ there exist positive constants B', a, b so that for $B>B'$

$$\int\mathring{\chi}_G^B P(d\varphi^{(k)})\leqslant\prod_{\Delta\in G}e^{2a-2bB^2(1+d(\Delta,J))}, \tag{2.15}$$

for any $G\subset Q_k$. This statement is also called the "Tail Lemma." The Main Lemma and Tail Lemma have been proven in Ref. 7 and adapted to the sine–Gordon problem in Refs. 2 and 3.

C. The Main Theorem and the result

Let us study the difference $\Delta^{(k)}[\mathscr{D}_k]$ [see (2.5)] more closely. We can imagine that the rough fields $\varphi^{(<k)}$ are the result of the rough fields $\varphi^{(j)}$ on scales $j=0,\ldots,k$ (Lemma 3.2, see Sec. III A) and that therefore the difference $\Delta^{(k)}[\mathscr{D}_k]$ can be bounded by a sum of contributions $F_k^{(j)}(\lambda,t)$ coming from the rough fields $\varphi^{(j)}$ for $j=0,\ldots,k$. That is, let us assume we have a bound of the following type (see Sec. III B), where $F_k^{(j)}$ is the $\varphi^{(j)}$-dependent contribution coming from scale k:

$$\Delta^{(k)}[\mathscr{D}_k]\leqslant\sum_{j=0}^{k}F_k^{(j)}(\lambda,t). \tag{2.16}$$

Furthermore, let us assume that we have integrated with respect to $P(d\varphi^{(h)})$ for $h=N,\ldots,k+1$ and that at each frequency we have been able to bound by a factor $\exp c(\lambda,h)$ anything dependent on the $\varphi^{(h)}$ fields but not integrable by the Main Lemma. This would mean that before integrating with respect to $P(d\varphi^{(k)})$ we would actually have the expression

$$\tilde{V}^{(k)}[\mathscr{D}_k^c]+\sum_{j=0}^{k}\sum_{h=k}^{N-2}(F_h^{(j)}(\lambda,t)+c(\lambda,h+1)) \tag{2.17}$$

in the exponent. Now the $F_h^{(k)}$, $h=k,\ldots,N-2$ are going to be the ones that are $\varphi^{(k)}$ dependent and will have to be estimated by an $\exp c(\lambda,k)$ factor. Note that $\Sigma_{j=0}^{N-1} F_{N-1}^{(j)}(\lambda,t)$ is set to zero since we know, e.g., by Ref. 1, Theorem 2.3 (this property was first proved in Ref. 3), that

$$\tilde{V}^{(N-1)}[\mathscr{D}_{N-1}]\leqslant 0, \tag{2.18}$$

allowing us to apply the Main Lemma for the $P(d\varphi^{(N-1)})$ integration immediately, taking care of the first steps in our recursive procedure. Hence we propose to prove the following theorem.

Theorem 2.1 ("Main Theorem"): For any given $\alpha^2 \in [4\pi,8\pi[$, $\lambda>0$, and $t\geqslant t_0(\alpha^2)$, here exist constants $c(\lambda,k)$, for $k=0,\ldots,N-2$, such that

$$\begin{aligned}\int \exp\left(\tilde{V}^{(k)}[\mathscr{D}_k^c]+\sum_{j=0}^{k}\sum_{h=k}^{N-2} F_h^{(j)}(\lambda,t)\right)P(d\varphi^{(k)})\\ \leqslant \exp c(\lambda,k)|\Lambda|\\ \times\exp\left(\tilde{V}^{(k-1)}[\mathscr{D}_{k-1}^c]\right.\\ \left.+\sum_{j=0}^{k-1}\sum_{h=k-1}^{N-2} F_{k-1}^{(j)}(\lambda,t)\right),\end{aligned} \tag{2.19}$$

where for $k=0$ it is understood that the second exponent on the rhs of (2.19) is missing.

The upper bound of ultraviolet stability is shown if the constants $c(\lambda,h)$ are summable in h, that is

$$c_+(\lambda):=\lim_{N\to\infty}\sum_{h=0}^{N-2} c(\lambda,h)<\infty. \tag{2.20}$$

Furthermore, it will be clear from the proof of Theorem 2.1 that

$$\lim_{\lambda\to 0} c_+(\lambda)\lambda^{-t+\tau}=0 \quad (\tau>0). \tag{2.21}$$

This proves the existence of the finite, positive constant $E_+(\lambda)$ independent of the volume $|\Lambda|$ and the cutoff N such that for all $\alpha^2\in[4\pi,8\pi[$, we have

$$\int e^{V^{(N)}[\Lambda]}p(d\varphi^{(<N)})\leqslant e^{E_+(\lambda)|\Lambda|}, \tag{2.22}$$

where $V^{(N)}[\Lambda]$ is the renormalized interaction defined in (1.7) with $E_+(\lambda)$ satisfying property (1.9).

III. THE PROOF OF THE MAIN THEOREM

A. Regions of large fluctuations and their properties

The heart of the proof will be to show that the large fluctuation contributions of the effective potentials (i.e., the parts integrated over regions of large fluctuations) give rise to a controllable remainder as the cutoff N is removed. The building blocks of the regions of large fluctuations, which we have already mentioned in Sec. II B, are the following two types of sets defined for all $k=0,\ldots,N$ and a fixed ϵ, $0<\epsilon\ll 1-\alpha^2/8\pi$ for a given $\alpha^2\in[4\pi,8\pi[$:

$$\begin{aligned}D^{(k)}:=D^{(k)}(B_k):=D^{(k)}(\varphi^{(<k)})\\ :=\{(\xi,\eta)\in\Lambda^2\,|\,|\sin^2((\alpha/2)(\varphi_\xi^{(<k)}-\varphi_\eta^{(<k)}))|\\ >B_k(\gamma^k|\xi-\eta|)^{1-\epsilon}\}\end{aligned} \tag{3.1}$$

and

$$\begin{aligned}R^{(k)}:=R^{(k)}(B_k):=R^{(k)}(\varphi^{(k)})\\ :=\{\Delta\in Q_k\,|\,\exists\xi\in\Delta,\eta\in\Lambda \text{ such that}\\ \gamma^k|\xi-\eta|<1 \text{ and}\\ |\sin((\alpha/2)(\varphi_\xi^{(k)}-\varphi_\eta^{(k)}))|\\ >(B_k/\sigma)(\gamma^k|\xi-\eta|)^{1-\epsilon}\\ \times(1+\gamma^k d(\Delta,\Lambda))\},\end{aligned} \tag{3.2}$$

where B_k is the strictly increasing succession defined as in (2.3) and $\sigma>1$ is a constant subsequently to be chosen sufficiently large. (Q_k is here a pavement of $\mathbb{R}^2$ consisting of tesserae with linear size γ^{-k}.)

We prove the following lemma.

Lemma 3.1: For all $k=0,\ldots,N$, we have

$$D^{(k)}\subseteq D^{(k-1)}\cup(R^{(k)}\times R^{(k)}), \tag{3.3}$$

$$(D^{(k)}\cap D^{(k-1)})\setminus(R^{(k)}\times R^{(k)})\subseteq D^{(k-1)}(B'_{k-1}), \tag{3.4}$$

with

$$B'_{k-1}:=\gamma^{1-2\epsilon}B_{k-1}, \tag{3.5}$$

for a fixed σ depending only on $\gamma>1$, $\alpha^2<8\pi$, and $\lambda>0$.

Proof: For (3.3) we show the converse, namely for $(\xi,\eta)\notin D^{(k-1)}\cup(R^{(k)}\times R^{(k)})$ follows $(\xi,\eta)\notin D^{(k)}$:

$$\begin{aligned}&(\xi,\eta)\notin D^{(k-1)}\\ &\Leftrightarrow|\sin(\alpha/2)(\varphi_\xi^{(<k-1)}-\varphi_\eta^{(<k-1)})|\\ &\qquad\leqslant B_{k-1}(\gamma^{k-1}|\xi-\eta|)^{1-\epsilon}\end{aligned}$$

and

$$(\xi,\eta)\notin R_k\times R_k \tag{3.6}$$

[and $(\xi,\eta)\in\Lambda^2$, otherwise the conclusion is obvious]

$$\begin{aligned}&\Rightarrow \text{either}|\sin((\alpha/2)(\varphi_\xi^{(k)}-\varphi_\eta^{(k)}))|\\ &\qquad\leqslant(B_k/\sigma)(\gamma^{(k)}|\xi-\eta|)^{1-\epsilon}\\ &\quad\text{or } \gamma^k|\xi-\eta|\geqslant 1\Rightarrow B_k(\gamma^k|\xi-\eta|)^{1-\epsilon}>1.\end{aligned} \tag{3.7}$$

The latter immediately implies $(\xi,\eta)\notin D^{(k)}$ while for the former we apply to the triangular inequality

$$\begin{aligned}&|\sin(\alpha/2)(\varphi_\xi^{(<k-1)}-\varphi_\eta^{(<k-1)})|\\ &\quad+|\sin(\alpha/2)(\varphi_\xi^{(k)}-\varphi_\eta^{(k)})|\\ &\geqslant|\sin(\alpha/2)(\varphi_\xi^{(<k)}-\varphi_\eta^{(<k)})|\end{aligned} \tag{3.8}$$

and thus

$$\begin{aligned}&\frac{B_{k-1}}{B_k\gamma^{1-\epsilon}}B_k(\gamma^k|\xi-\eta|)^{1-\epsilon}+\frac{B_k}{\sigma}(\gamma^k|\xi-\eta|)^{1-\epsilon}\\ &\geqslant|\sin(\alpha/2)(\varphi_\xi^{(<k)}-\varphi_\eta^{(<k)})|,\end{aligned} \tag{3.9}$$

which implies $(\xi,\eta)\notin D^{(k)}$ as well since we can pick a finite $\sigma_1(\theta_1)$ large enough so that for any θ_1, with $\gamma^{-(1-\epsilon)}<\theta_1<1$,

$$\begin{aligned}&B_{k-1}/B_k\gamma^{1-\epsilon}+1/\sigma\leqslant\theta_1,\\ &\quad\text{for all } k=0,\ldots,N \text{ and all } \sigma>\sigma_1(\theta_1).\end{aligned} \tag{3.10}$$

Inclusion (3.4) is proved using the triangular inequality (3.8) in the other direction and noting that for $(\xi,\eta)\in(D^{(k)}\cap D^{(k-1)})\setminus(R^{(k)}\times R^{(k)})$:

$$(\xi,\eta)\in D^{(k)}$$
$$\Leftrightarrow|\sin(\alpha/2)(\varphi_{\xi}^{(<k)}-\varphi_{\eta}^{(<k)})|$$
$$>B_k(\gamma^k|\xi-\eta|)^{1-\epsilon}, \tag{3.11}$$
$$(\xi,\eta)\notin R^{(k)}\times R^{(k)}$$
$$\Rightarrow|\sin(\alpha/2)(\varphi_{\xi}^{(k)}-\varphi_{\eta}^{(k)})|$$
$$\leqslant(B_k/\sigma)(\gamma^k|\xi-\eta|)^{1-\epsilon}. \tag{3.12}$$

Thus we have

$$|\sin(\alpha/2)(\varphi_{\xi}^{(<k-1)}-\varphi_{\eta}^{(<k-1)})|$$
$$\geqslant B_k(\gamma^k|\xi-\eta|)^{1-\epsilon}-\frac{B_k}{\sigma}(\gamma^k|\xi-\eta|)^{1-\epsilon}$$
$$\geqslant(B_k/B_{k-1})(1-1/\sigma)\gamma^{1-\epsilon}B_{k-1}(\gamma^{k-1}|\xi-\eta|)^{1-\epsilon}$$
$$\geqslant\gamma^{1-2\epsilon}B_{k-1}(\gamma^{k-1}|\xi-\eta|)^{1-\epsilon}, \tag{3.13}$$

provided we pick a finite

$$\sigma>\sigma_2(\epsilon)\geqslant\gamma^{\epsilon}/(\gamma^{\epsilon}-1), \tag{3.14}$$

so that $(1-1/\sigma)\geqslant\gamma^{-\epsilon}$. Picking a σ greater than $\max\{\sigma_1(\theta_1),\sigma_2(\epsilon)\}$ completes the proof.

Figure 1 illustrates the statement of Lemma 3.1. ■

Lemma 3.2: Define $B(k,h):=\gamma^{(1-2\epsilon)(k-h)}B_{k-h}$ for all $k\geqslant h\geqslant 0$. Then we have the following inclusion for all $k=0,\ldots,N$:

$$D^{(k)}(\varphi^{(<k)})\subseteq\bigcup_{h=0}^{k}R^{(h)}(B(k,h);\varphi^{(h)})^2. \tag{3.15}$$

Proof: By applying (3.3) of Lemma 3.1 onto the disjoint union

$$D^{(k)}=(D^{(k)}\setminus D^{(k-1)})\cup(D^{(k)}\wedge D^{(k-1)})$$
$$\subseteq(R^{(k)}\times R^{(k)})\cup[(D^{(k)}\cap D^{(k-1)})\setminus(R^{(k)}\times R^{(k)})] \tag{3.16}$$

and then iterating using (3.4) upon the square brackets in the rhs of (3.16) we get

$$D^{(k)}(B_k)\subseteq R^{(k)}(B_k)^2\cup D^{(k-1)}(B'_{k-1})$$
$$\subseteq R^{(k)}(B_k)^2\cup R^{(k-1)}(B'_{k-1})^2$$
$$\cup D^{(k-2)}(B''_{k-2}), \tag{3.17}$$

which terminates after $k+1$ steps since $D^{(-1)}\equiv\emptyset$. Introducing the new notation for the B primes proves the assertion. ■

B. An upper bound for $\Delta^{(k)}[\mathscr{D}_k]$

For Theorem 2.2 in Ref. 1 we know that the terms of order $n\geqslant 2$ and λ for $\Delta^{(k)}[\mathscr{D}_k]$ may be estimated proportional to

$$\gamma^{2k}\lambda_{\text{eff}}^{n}(k)\int_{D^{(k)}}d\xi\,d\eta\,\sin^2\frac{\alpha}{2}(\varphi_{\xi}^{(<k)}-\varphi_{\eta}^{(<k)}). \tag{3.18}$$

Estimating the integrand by 1 and applying the decomposition (3.15) of Lemma 3.2 for $D^{(k)}$ we have the following estimate (A a positive constant):

$$\Delta^{(k)}[\mathscr{D}_k]\leqslant\sum_{n=3}^{t}\sum_{j=0}^{k}A\lambda_{\text{eff}}^{n}(k)\gamma^{2k}|R^2(k,j)|$$
$$=:\sum_{j=0}^{k}F_k^{(j)}(\lambda,t)$$
$$=\sum_{j=0}^{k}\left\{A\gamma^{2k}|R^2(k,j)|\sum_{n=3}^{t}\lambda_{\text{eff}}^{n}(k)\right\}, \tag{3.19}$$

where

$$|R^2(k,j)|:=\int_{(R^{(j)}(B(k,j);\varphi^{(j)}))^2}d\xi\,d\eta, \tag{3.20}$$

depending on the field $\varphi^{(j)}$. Note that second-order terms are missing in (3.19) since they are negative (Theorem 2.3 in Ref. 1).

C. The proof completed

Let $\chi_{\Delta}^{\overline{B}(h,k)}$ be the characteristic function of $E_{\Delta}^{\overline{B}(h,k)}$ [defined as in (2.9)], where $(h\geqslant k>0)$:

$$\overline{B}(h,k):=(1/\sigma)B(h,k)=(1/\sigma)\gamma^{(1-2\epsilon)(h-k)}B_{h-k}, \tag{3.21}$$

as in Lemma 3.2. Let $G_k\supseteq G_{k+1}\supseteq\cdots\supseteq G_N\supseteq G_{N+1}:=\emptyset$ be a chain of arbitrary sets of squares in the pavement Q_k of $\mathbb{R}^2$. Writing

$$\chi_{G_h\setminus G_{h+1}}^{\overline{B}(h,k)}:=\prod_{\Delta\in G_h\setminus G_{h+1}}\chi_{\Delta}^{\overline{B}(h,k)} \tag{3.22}$$

and $\mathring{\chi}$ analogously as in (2.11), and observing that

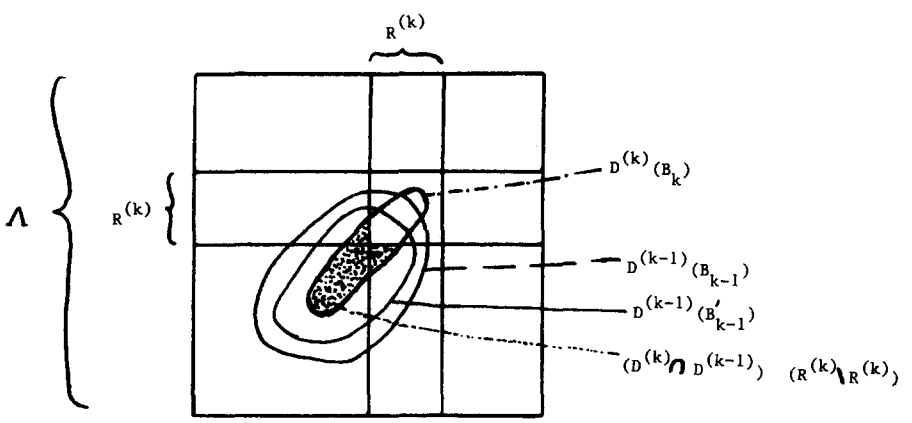

FIG. 1. The sets of large fluctuations.

$$G_k \equiv \bigcup_{h=k}^{N} (G_h \setminus G_{h+1}),$$

we can immediately write the following decomposition of the identity:

$$1 \equiv \sum_{\tilde{G}} \chi_{Q_k \setminus G_k}^{\bar{B}(k,k)} \mathring{\chi}_{G_k \setminus G_{k+1}}^{\bar{B}(k,k)} \cdots \mathring{\chi}_{G_h \setminus G_{h+1}}^{\bar{B}(h,k)} \cdots \mathring{\chi}_{G_N}^{\bar{B}(N,k)}, \quad (3.23)$$

where the sum runs over all possible chains $\tilde{G}$ in Q_k.

Calling I the lhs of (2.19), which is the integral we want to estimate in the Main Theorem, we use this decomposition of the identity and obtain

$$\begin{aligned} I &:= \int \exp\left(\tilde{V}^{(k)}[\mathscr{D}_k^c] + \sum_{j=0}^{k} \sum_{h=k}^{N-2} F_h^{(j)}(\lambda,t)\right) P(d\varphi^{(k)}) \\ &= \sum_{\tilde{G}} \int \exp(\tilde{V}^{(k)}[\mathscr{D}_k^c]\, \chi_{Q_k \setminus G_k}^{\bar{B}(k,k)}) \\ &\quad \times \left(\exp\left(\sum_{j=0}^{k} \sum_{h=k}^{N-2} F_h^{(j)}(\lambda,t)\right)\right. \\ &\quad \left. \times \mathring{\chi}_{G_k \setminus G_{k+1}}^{\bar{B}(k,k)} \cdots \mathring{\chi}_{G_N}^{\bar{B}(N,k)}\right) P(d\varphi^{(k)}). \end{aligned} \quad (3.24)$$

The crucial observation now is that the sets $R^2(h,k)$ themselves build a chain since for all $h \geqslant h' \geqslant k$, $\bar{B}(h',k) \leqslant \bar{B}(h,k)$ and thus

$$\begin{aligned} R^2(h,k) &\supseteq R^2(k+1,k) \supseteq \cdots \supseteq R^2(h',k) \\ &\supseteq \cdots \supseteq R^2(h,k) \supseteq \cdots \supseteq R^2(N,k). \end{aligned} \quad (3.25)$$

Defining $R^2(N+1,k) := \varnothing$ for all k, we can write the following identity for all $h \geqslant k$:

$$R^2(h,k) = \bigcup_{l=h}^{N} (R^2(l,k) \setminus R^2(l+1,k)), \quad (3.26)$$

whence it is clear that for a given $\gamma\varphi^{(k)}$ there is some chain $\tilde{G}$ with

$$\mathring{\chi}_{G_k \setminus G_{k+1}}^{\bar{B}(k,k)} \cdots \mathring{\chi}_{G_j \setminus G_{j+1}}^{\bar{B}(j,k)} \cdots \mathring{\chi}_{G_N}^{\bar{B}(N,k)} \varphi^{(k)} = 1. \quad (3.27)$$

The contribution to $|R^2(h,k)|$ in $F_h^{(k)}(\lambda,t)$ [see (3.19)] comes from a sum $\Sigma_{l=h}^{N} |R^2(l,k) \setminus R^2(l+1,k)|$, which will be the same for the chain $\tilde{G}$: $\Sigma_{l=h}^{N} |G_l \setminus G_{l+1}|$, now field independent. Taking this into account we can bound the last $\varphi^{(k)}$-dependent term in the double sum of the rhs of (3.24) as follows:

$$\begin{aligned} \sum_{j=0}^{k} \sum_{h=k}^{N-2} F_h^{(j)}(\lambda,t) &\leqslant \sum_{j=0}^{k-1} \sum_{h=k}^{N-2} F_h^{(j)}(\lambda,t) + \sum_{h=k}^{N-2} \sum_{l=h}^{N} A\gamma^{2h} |R^2(l,k) \setminus R^2(l+1,k)| \sum_{n=3}^{t} \lambda_{\mathrm{eff}}^{n}(h) \\ &\leqslant \sum_{j=0}^{k-1} \sum_{h=k}^{N-2} F_h^{(j)}(\lambda,t) + \sum_{h=k}^{N} \sum_{l=k}^{h} \sum_{n=3}^{t} A' \lambda_{\mathrm{eff}}^{n}(l) \gamma^{2l} |G_h \setminus G_{h+1}|, \end{aligned} \quad (3.28)$$

where we have exchanged the double sum $\Sigma_{h=k}^{N-2} \Sigma_{l=h}^{N}(h,l)$ by $\Sigma_{p=k}^{N} \Sigma_{q=k}^{p}(h \to q, l \to p)$ (setting to zero some of the terms in the latter sum) and then renamed p and q back to k and l. The l-dependent part in (3.28) is proportional to

$$\gamma^{(\alpha^2/4\pi - 2)nl + 2l} = \gamma^{2nl(\alpha^2/8\pi - (1-1/n))} \begin{cases} > 1, & \text{for } n \leqslant t_0(\alpha^3), \\ < 1, & \text{for } n > t_0(\alpha^2), \end{cases} \quad (3.29)$$

since $t_0(\alpha^2)$ had been chosen as such (see Sec. I B). Thus, for $n > t_0$ the sum over l in (3.28) is proportional to the first term while for $n \leqslant t_0$ we bound the sum over l by the largest (last) term of the sum times $(h-k+1)$, that is, the number of terms in this sum. Therefore, we get

$$\begin{aligned} \sum_{j=0}^{k} \sum_{h=k}^{N-2} F_h^{(j)}(\lambda,t) &\leqslant \sum_{j=0}^{k-1} \sum_{h=k}^{N-2} F_h^{(j)}(\lambda,t) \\ &\quad + \sum_{h=k}^{N} \left[\sum_{n=3}^{t_0} A_0(h-k+1) \lambda_{\mathrm{eff}}^{n}(h) \gamma^{2h} |G_h \setminus G_{h+1}| + \sum_{n=t_0+1}^{t} A_1 \lambda_{\mathrm{eff}}^{n}(k) \gamma^{2k} |G_h \setminus G_{h+1}| \right]. \end{aligned} \quad (3.30)$$

Using the Main Lemma to estimate I with (3.30) introduced into (3.24), we have

$$\begin{aligned} I &\leqslant \exp(\delta(B_k, \lambda_{\mathrm{eff}}(k)) \gamma^{2k} |\Lambda|) \exp(\tilde{V}^{(k-1)}[\mathscr{D}_{k-1}^c] + \Delta^{(k-1)}[\mathscr{D}_{k-1}]) \\ &\quad \times \sum_{\tilde{G}} \left\{ \exp(\bar{A} \lambda_{\mathrm{eff}}(k) B_k^{2+g} \gamma^{2k} |G_k \cap \Lambda| + (3.30)) \left[\int P(d\varphi^{(k)}) \mathring{\chi}_{G_k \setminus G_{k+1}}^{\bar{B}(k,k)} \cdots \mathring{\chi}_{G_N}^{(N,k)} \right]^{1/2} \right\}. \end{aligned} \quad (3.31)$$

We are now left to show that $\Sigma_{\tilde{G}}\{\cdots\}$ is summable in k, that is, that it can be incorporated into the remainder. Note that $\Delta^{(k-1)}[\mathscr{D}_{k-1}]$, contributes a new $\Sigma_{j=0}^{k-1} F_{k-1}^{(j)}(\lambda,t)$, which combines with the first term on the rhs of (3.30) reproducing the expression we had on scale k but now for scale $k-1$. Applying a "refined version" of the Tail Lemma (see Sec. II B and Ref. 2) we obtain

$$[\cdots]^{1/2} \leqslant \prod_{h=k}^{N} \prod_{\Delta \in G_h \setminus G_{h+1}} \exp(a - b\bar{B}^2(h,k))(1 + \gamma^{2k} d(\Delta,\Lambda)) \quad (3.32)$$

Noting that

$$e^{|G_h \setminus G_{h+1}|} = \prod_{\Delta \in G_h \setminus G_{h+1}} e^{|\Delta|} \quad (|\Delta| = \gamma^{-2k}),$$

we pull down the sums over h in (3.30) and write them as the product of the exponentials in $\Sigma_{\tilde{G}}$ and obtain for this sum in

(3.31) the following ($g' > g$, other constants chosen appropriately):

$$\sum_{\bar{G}} \prod_{h=k}^{N} \prod_{\Delta \in G_h \setminus G_{h+1}} \left\{ \exp\left[a + \bar{A}\lambda_{\text{eff}}(k) B_k^{2+g'} + \sum_{n=3}^{t_0} A_0' h \lambda_{\text{eff}}^n(h) \gamma^{2(h-k)} \right.\right.$$
$$\left.\left. + \sum_{n=t_0+1}^{t} A_1' \lambda_{\text{eff}}^n(k) - b\bar{B}^2(h,k)(1+\gamma^{2k} d(\Delta,\Lambda)) \right] \right\}. \tag{3.33}$$

Estimating this as a product of squares,

$$\prod_{\Delta \in Q_k} \left\{ 1 + \sum_{h=k}^{N} \exp\left[a + \bar{A}\lambda_{\text{eff}}(k) B_k^{2+g'} + \sum_{h=t_0+1}^{t} A_1' \lambda_{\text{eff}}^n(k) \right.\right.$$
$$\left.\left. + \sum_{n=3}^{t_0} A_0' h \lambda_{\text{eff}}^n(h) \gamma^{2(h-k)} - b\bar{B}^2(h,k)(1+\gamma^{2k} d(\Delta,\Lambda)) \right] \right\}, \tag{3.34}$$

we note that the sum over n from 3 to t_0 is the only dangerous term; however, for h sufficiently large, the negative term overrides since the ratio

$$\frac{\bar{B}^2(h,k)}{h\gamma^{(\alpha^2/4\pi - 2)nh}\gamma^{2(h-k)}} = \frac{\gamma^{2(1-2\epsilon)(h-k)} B_{h-k}^2}{\sigma^2 h \gamma^{(\alpha^2/4\pi - 2)nh}\gamma^{2(h-k)}} \geqslant (\text{const}/h)\gamma^{4h((1-\alpha^2/8\pi)(n/2)-\epsilon)}, \tag{3.35}$$

and the last expression can be made to be greater than 1 for any $n \geqslant 3$ by choosing $\epsilon \ll 1 - \alpha^2/8\pi$ and requiring h to be sufficiently large, i.e., greater than some frequency k_0. The effective potential at this frequency k_0 will not give rise to ultraviolet problems anymore since now only a finite number of integrations has to be performed. Nevertheless, as λ goes to zero, we can choose k_0 to be 1 as well. The product (3.34) thus can be estimated by

$$\exp(\bar{c}\exp(-\bar{b}B^2)\gamma^{2k}|\Lambda|), \tag{3.36}$$

with $\bar{c}$ and $\bar{b}$ appropriately chosen. By adjusting D in the definition of δ (see Sec. II B) we note that (3.36) has the form

$$\exp(\delta\gamma^{2k}|\Lambda|),$$

which completes the proof. ■

Note added in proof: The techniques presented in this paper also can be used in order to prove the asymptoticity of the Mayer series for the pressure in the corresponding Coulomb gas problem [cf. Refs. 8 and 9]. We are grateful for the possibility we have had to thoroughly discuss this extension of our results with Francesco Nicolò during a stay at the I.H.E.S. in Bures-sur-Yvette, France.

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Two-loop counterterms for the Wess–Zumino model on anti-de Sitter space

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The two-loop counterterms for the Wess–Zumino model on a four-dimensional anti-de Sitter space background are computed. It is shown that, as at the one-loop level, the counterterms preserve supersymmetry but the nonrenormalization theorem is violated by the addition of a divergent linear term to the superpotential.

I. INTRODUCTION

Recently the subject of supersymmetric field theories defined on a curved anti-de Sitter (AdS) space background has proved an interesting and fruitful field of investigation.[1–10] Motivation is provided by the appearance of AdS space in the maximally supersymmetric classical solutions of supergravity theories.[11] Moreover, when quantized, supersymmetric field theories on AdS space have been shown to evince properties strikingly different to their flat-space counterparts. The purpose of the present work is to explore further the most noteworthy deviation from flat-space behavior so far discovered; namely the failure of the nonrenormalization theorem for the Wess–Zumino model on a four-dimensional AdS background.[9]

First, however, let us summarize the previous development of the subject, concentrating on four-dimensional anti-de Sitter space $(AdS)_4$.

Burgess[5] calculated the vacuum energy to one-loop order for a general field theory on an $(AdS)_4$ background, demonstrating the preservation of supersymmetry to one-loop order and obtaining the one-loop corrections to the radius of the $(AdS)_4$ space. Burges *et al.*[7] discussed the Wess–Zumino model on an $(AdS)_4$ background and showed how to obtain conserved generators for the isometry group $O(3,2)$, having a manifestly positive energy density and vanishing expectation value in a supersymmetric vacuum.

Two groups of authors[8–10] have calculated the one-particle-irreducible one- and two-point functions to one-loop order for the Wess–Zumino model on $(AdS)_4$. The normal coordinate momentum space expansion for propagators in curved space-time, developed by Bunch and Parker,[12] played an important role in these computations. Düsedau and Freedman,[9] using a manifestly supersymmetric Pauli–Villars regularization scheme, found that the auxiliary field had a vanishing vacuum expectation value, consistent with the preservation of supersymmetry to this order. However, they found the scalar field to acquire a divergent vacuum expectation value and concluded that the nonrenormalization theorem,[13] which states that the classical superpotential is not renormalized by quantum corrections, is violated by the Wess–Zumino model on the $(AdS)_4$ background.

In addition to using the Pauli–Villars scheme, Bellucci and Gonzalez[8] proposed as a candidate for a supersymmetric regularization scheme on the $(AdS)_4$ background a variant of dimensional regularization in which the curvature tensor is assumed to have strictly four-dimensional indices while all other quantities are analytically continued away from four dimensions.

In the present paper we shall extend the results of Düsedau and Freedman[9] to the two-loop level. If we restrict ourselves to the consideration of divergences, it proves possible to apply the modified dimensional regularization scheme suggested by Bellucci and Gonzalez[8] even at two loops. We use the background field method[14,15]; in this context the divergences of the one-loop effective action may be efficiently evaluated using the well-known Schwinger–DeWitt kernel techniques, confirming the results of Düsedau and Freedman.[9] The two-loop effective action is written as the sum of vacuum graphs in the presence of background scalar, auxiliary, and fermion fields. The background-dependent propagators may be expressed in terms of Green's functions for second-order differential operators. Such Green's functions may be expanded as a series in which singular, purely space-time-dependent quantities multiply coefficients derived from the standard asymptotic expansion of the Schwinger–DeWitt kernel for the operator in question.[16] Ultraviolet divergences arise from the products of these singular functions, which occur when the expansion for the Green's function is inserted into the expression for a Feynman graph. All potentially divergent products of these singular functions, together with the resulting divergences, have been tabulated elsewhere.[16] It is therefore relatively straightforward to calculate the two-loop counterterms for the Wess–Zumino model on the $(AdS)_4$ background in a systematic fashion. We find that they take a precisely similar form to the one-loop counterterms. To be specific, we find a term of the same form as the original kinetic part of the Lagrangian together with terms that correspond to adding a divergent term, linear in the scalar field, to the superpotential in the interaction Lagrangian. We deduce that at the two-loop level supersymmetry is preserved by the divergent counterterms, but the nonrenormalization theorem fails, exactly as at one loop.

The paper is organized as follows: In Sec. II we define the Wess–Zumino model on $(AdS)_4$. We introduce the Schwinger–DeWitt kernel, use it to compute the one-loop counterterms, and discuss the consequences. In Sec. III we recapitulate the general procedure for computing two-loop divergences using the Schwinger–DeWitt kernel and use it to evaluate the two-loop counterterms for our model. In Sec. IV we summarize our results and offer some concluding remarks.

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II. ONE-LOOP CALCULATION

Anti-de Sitter space in four dimensions $(AdS)_4$ is the hyperboloid $\eta_{AB}\, y^A y^B = a^{-2}$ embedded in R^5 with Cartesian coordinates y^A and flat metric $\eta_{AB} = (+,-,-,-,+)$. Full details of the geometry are given elsewhere[17,18]; from our point of view the important result is the expression for the curvature tensor

$$R_{\mu\nu\alpha\beta} = a^2(g_{\mu\beta}\, g_{\nu\alpha} - g_{\mu\alpha}\, g_{\nu\beta})\,. \tag{2.1}$$

We also assume the existence of a set of vierbein fields $e^a{}_\mu$, where the index a refers to a local Minkowski frame. We have, for $e^a{}_\mu$ and its inverse $e_a{}^\mu$,

$$g_{\mu\nu} = e^a{}_\mu e^b{}_\nu \eta_{ab}\,, \quad \eta_{ab} = e_a{}^\mu e_b{}^\nu g_{\mu\nu}\,, \tag{2.2}$$

and we introduce flat γ-matrices γ^a in the local frame, satisfying

$$\{\gamma^a,\gamma^b\} = 2\eta^{ab}\,, \quad \{\gamma_5,\gamma^a\} = 0\,, \quad \gamma_5{}^2 = 1\,. \tag{2.3}$$

We define γ-matrices γ_μ in an arbitrary frame by

$$\gamma_\mu = e^a{}_\mu \gamma_a\,. \tag{2.4}$$

Although we shall use dimensional regularization[19] so that all quantities are regarded as extended to d dimensions (with $d = 4-\epsilon$) we shall adopt the suggestion of Bellucci and Gonzalez[8] and consider the indices of $R_{\mu\nu\alpha\beta}$ in (2.1) as strictly four-dimensional, so that we still have the exact relations

$$R_{\mu\nu} = -3a^2 g_{\mu\nu}\,, \quad R = -12a^2\,. \tag{2.5}$$

Moreover we shall assume (2.3) to remain valid for $d \neq 4$. There appear to be no contradictions provided no strictly four-dimensional γ-matrix completeness or index identities are assumed.

The Wess–Zumino model on $(AdS)_4$ is defined by the following action[20]:

$$S[z,z^\dagger,F,F^\dagger,\chi,\bar\chi] = S_{\rm kin}[z,z^\dagger,F,F^\dagger,\chi,\bar\chi] + S_{\rm int}[z,z^\dagger,F,F^\dagger,\chi,\bar\chi]\,, \tag{2.6}$$

where

$$S_{\rm kin} = \int dv_x \{\partial^\mu z^\dagger Z_S\, \partial_\mu z + i\bar\chi Z_F \not\nabla \chi + F^\dagger Z_A F + a(z^\dagger Z_{SA} F + F^\dagger Z_{SA} z) + 3a^2 z^\dagger Z_Q z\}\,, \tag{2.7a}$$

$$S_{\rm int} = \mu^{-\epsilon}\int dv_x \left\{\bar w_B{}^{,a}\bar F_a + w_{B,a}F^a - \frac{1}{2}\bar w_B{}^{,ab}\bar\chi_a\chi'_b - \frac{1}{2}w_{B,ab}\bar\chi'^a\chi^b + 3a(\bar w_B + w_B)\right\}. \tag{2.7b}$$

Here z is a vector of n complex scalar fields z^a, and its Hermitian conjugate $z^\dagger$ has components $z^\dagger_a = (z^a)^*$. Also F is a vector of n complex auxiliary fields F^a and its Hermitian conjugate $F^\dagger$ has components $F^\dagger_a = (F^a)^*$; and χ is a vector of n right-handed spinor fields χ^a with $\gamma_5\chi^a = \chi^a$ and $\bar\chi$ is the conjugate with components $\bar\chi_a = \overline{\chi^a}$ so that $\bar\chi_a\gamma_5 = -\bar\chi_a$. We may then regard (z,χ,F) and $(z^\dagger,\bar\chi,F^\dagger)$ as independent chiral multiplets. Introducing the charge conjugation matrix C satisfying

$$C^T = -C\,, \quad (C\gamma_a)^T = C\gamma_a\,, \quad (C\gamma_5)^\dagger = -C\gamma_5\,, \tag{2.8}$$

we define χ' by

$$\chi'_a = C\bar\chi_a^T\,, \tag{2.9}$$

so that χ'_a is left handed. From our point of view, since $\mathrm{tr}(\frac{1}{2}(1\pm\gamma_5)) = 2$ we can regard χ,χ' as being effectively left- and right-handed two-component spinors. We use $\not\nabla$ to denote $\gamma_\mu\nabla^\mu$. We assume that ∇^μ always contains the appropriate metric connection for the quantity on which it acts.

In (2.7b), $w_B(z)$ is the bare superpotential and $\bar w_B(z^\dagger)$ its complex conjugate. Now $w_B(z)$ may be written as

$$w_B(z) = (\mu^{(3/2)\epsilon}/3!)\lambda_{Babc}z^a z^b z^c + (\mu^\epsilon/2)\kappa_{Bab}z^a z^b + \mu^{(1/2)\epsilon}\nu_{Ba}z^a + \rho_B \tag{2.10}$$

and

$$\bar w^a = \frac{\partial\bar w}{\partial z^\dagger_a}\,, \quad w_{,a} = \frac{\partial w}{\partial z^a}\,. \tag{2.11}$$

In (2.7a) we have inserted renormalization matrices Z_S, Z_F, Z_A, Z_{SA}, and Z_Q, which, together with the bare parameters λ_B, κ_B, ν_B, and ρ_B in (2.10), provide counterterms necessary for renormalizability when the theory is quantized. Finally, dv_x is the invariant integration measure on $(AdS)_4$ and μ is the dimensional regularization unit of mass.[21]

The kinetic and interaction actions in (2.7) are separately invariant under the supersymmetry transformations

$$\delta z = \bar\epsilon_+\chi\,, \tag{2.12a}$$

$$\delta\chi = F\epsilon_+ - i\not\partial z\epsilon_-\,, \tag{2.12b}$$

$$\delta\bar\chi = \bar\epsilon_+ i\not\partial z^\dagger + F^\dagger\epsilon_-\,, \tag{2.12c}$$

$$\delta F = -\bar\epsilon_- i\not\nabla\chi - \bar\epsilon_+ a\chi\,, \tag{2.12d}$$

where ϵ_+ and ϵ_- are the right- and left-handed components, respectively, of a Killing spinor ϵ satisfying

$$\nabla_\mu\epsilon(x) = -(ia/2)\gamma_\mu\epsilon(x) \tag{2.13}$$

and $\bar\epsilon_+ = \overline{\epsilon_-}$, $\bar\epsilon_- = \overline{\epsilon_+}$.

We shall use the background field method[14,15] so that, in the functional integral defining the quantum theory, the quantum fields denoted z^q, χ^q, F^q (and their conjugates) are expanded about arbitrary classical background fields z,χ,F, and their conjugates, according to

$$z^q = z + y\,, \quad F^q = F + f\,, \quad \chi^q = \chi + \eta\,. \tag{2.14}$$

It is convenient to assemble the fluctuation fields y,f,η, and their conjugates into a single column vector V, with conjugate $\bar V$, given by

$$V = \begin{pmatrix} y \\ y^* \\ f \\ f^* \\ \eta \\ \eta' \end{pmatrix}, \quad \bar V = (y^\dagger\, y^T f^\dagger f^T \bar\eta\ \bar\eta')\,, \tag{2.15}$$

where V and $\bar V$ satisfy a Majorana-like condition

$$\bar V = V^T\mathscr{C}\,,$$

$$\mathscr{C} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \otimes \begin{pmatrix} \mathbb{1}_2 & 0 & 0 \\ 0 & \mathbb{1}_2 & 0 \\ 0 & 0 & -C^{-1} \end{pmatrix}. \tag{2.16}$$

The notation in (2.16) means that each entry in the right-hand matrix is multiplied by the left-hand matrix, $\mathbf{1}_2$ is the unit matrix in two dimensions, and C is as defined in (2.8).

There is a natural scalar product

$$(\bar{V}_1,V_2)=(\bar{V}_2,V_1)$$
$$=\int dv_x\{y_1^\dagger y_2+y_2^\dagger y_1+f_1^\dagger f_2+f_2^\dagger f_1$$
$$+\bar{\eta}_1\eta_2+\bar{\eta}_2\eta_1\}. \tag{2.17}$$

The quantum field theory may be defined by the connected vacuum functional $W[z,z^\dagger,F,F^\dagger,\chi,\bar{\chi},K]$ with a source K coupled only to the quantum fluctuation vector

$$\exp\left(\frac{iW}{\hbar}\right)$$
$$=\int d[V]\exp\left\{\frac{i}{\hbar}(S[z^q,z^{q\dagger},F^q,F^{q\dagger},\chi^q,\bar{\chi}^q]+(K,V)\right\}, \tag{2.18}$$

where S is as given by (2.6).

The renormalization constants in $S_{\rm kin}$ and the bare coupling constants λ_B, κ_B, ν_B, and ρ_B in $S_{\rm int}$ are written as expansions in $\hbar$:

$$Z_{S,F,A,SA,Q}=1+\sum_{n=1}^{\infty}\hbar^n Z^{(n)}_{S,F,A,SA,Q},$$
$$\lambda_B=\lambda+\sum_{n=1}^{\infty}\hbar^n\lambda^{(n)},$$
$$\kappa_B=\kappa+\sum_{n=1}^{\infty}\hbar^n\kappa^{(n)}, \tag{2.19}$$
$$\nu_B=\nu+\sum_{n=1}^{\infty}\hbar^n\nu^{(n)},$$
$$\rho_B=\rho+\sum_{n=1}^{\infty}\hbar^n\rho^{(n)}.$$

The coefficients of $\hbar^n$ in (2.19) are chosen so that W in (2.18) is finite order by order in the perturbation expansion. We adopt the minimal subtraction prescription[21] so that the coefficients are fixed uniquely by requiring they contain only poles in ϵ. We use the notation $S^{(n)}$ to denote the $O(\hbar^n)$ contribution to S in (2.6). Henceforth we suppress $\hbar$. We write the renormalized superpotential w as

$$w=(\mu^{(3/2)\epsilon}/3!)\lambda_{abc}z^az^bz^c$$
$$+(\mu^\epsilon/2!)\kappa_{ab}z^az^b+\mu^{(1/2)\epsilon}\nu_az^a+\rho, \tag{2.20}$$

where λ, κ, ν, and ρ are as in (2.19). The one-loop contribution to W is generated by the quadratic fluctuations in the exponent of (2.18). We have

$$S[z^q,z^{q\dagger},F^q,F^{q\dagger},\chi^q,\bar{\chi}^q]$$
$$=S[z,z^\dagger,F,F^\dagger,\chi,\bar{\chi}]$$
$$+(J,V)-\tfrac{1}{2}(\bar{V},\Delta_V^B V)+S_I[V,\bar{V}], \tag{2.21}$$

where Δ_V^B has the form

$$\Delta_V^B=\begin{pmatrix}\Delta_z^B & -\mathscr{M}_B & \bar{\mathscr{F}}_B\\ -\mathscr{M}_B & -\mathbf{1}_2 & 0\\ \mathscr{F}_B & 0 & d_B\end{pmatrix}, \tag{2.22}$$

with

$$\mathscr{M}_B=\begin{pmatrix}a & \bar{M}_B\\ M_B & a\end{pmatrix}, \tag{2.23a}$$

$$\mathscr{F}_B=\begin{pmatrix}0 & \Lambda^{B'}\\ \Lambda^B & 0\end{pmatrix},\quad \bar{\mathscr{F}}_B=\begin{pmatrix}0 & \bar{\Lambda}^B\\ \bar{\Lambda}^{B'} & 0\end{pmatrix}, \tag{2.23b}$$

where

$$M_{Bab}=\mu^{-\epsilon}w_{B,ab},\quad \bar{M}_B^{ab}=\mu^{-\epsilon}\bar{w}_B^{ab},\quad \Lambda^B_{ab}=\mu^{(1/2)\epsilon}\lambda_{Babc}\chi^c. \tag{2.24}$$

The scalar and fermion operators Δ_z^B and d_B are defined by

$$\Delta_z^B=\Box\mathbf{1}_2-\mathscr{V}_B,\quad d_B=(-i\not{\partial}+\mathscr{N}_B)\mathbf{1}_2, \tag{2.25a}$$

$$\mathscr{V}_B=\begin{pmatrix}3a^2 & \bar{K}_B+3a\bar{M}_B\\ K_B+3aM_B & 3a^2\end{pmatrix},$$

$$\mathscr{N}=\begin{pmatrix}0 & \bar{M}_B\\ M_B & 0\end{pmatrix}, \tag{2.25b}$$

$$K_{Bab}=\mu^{(1/2)\epsilon}\lambda_{Babc}F^c. \tag{2.25c}$$

Here, $S_I[V,\bar{V}]$ consists of terms cubic in the fluctuations that provide interactions at two- and higher-loop order. It will be given explicitly in the next section. We choose the source K in (2.18) to cancel the linear term (J,V) in the expansion (2.21).

To one loop, (2.18) and (2.21) yield

$$W^{(1)}[z,z^\dagger,F,F^\dagger,\chi,\bar{\chi}]$$
$$=S^{(1)}[z,z^\dagger,F,F^\dagger,\chi,\bar{\chi}]+(i/2)\ln(\operatorname{sdet}\Delta_V), \tag{2.26}$$

where Δ_V is obtained by replacing all quantities in (2.22) by their renormalized counterparts. The superdeterminant sdet in (2.26) appears as a consequence of integration over the anticommuting variables $\eta,\bar{\eta}$ and is defined as follows, for a matrix

$$X=\begin{pmatrix}A & B\\ C & D\end{pmatrix}$$

acting on a space containing both bosonic and fermionic degrees of freedom:

$$\operatorname{sdet}X=\det(A-BD^{-1}C)(\det D)^{-1}. \tag{2.27}$$

The supertrace is correspondingly defined by

$$\operatorname{str}X=\operatorname{tr}A-\operatorname{tr}D. \tag{2.28}$$

We intend to use the Schwinger–De Witt kernel to investigate the singular behavior of sdet Δ_V. From this point of view Δ_V has the disadvantage that it is not second order in derivatives in the fermionic and auxiliary sectors. To circumvent this obstacle we write[22]

$$\Delta_W=\Delta_L\,\Delta_V\,\Delta_R, \tag{2.29}$$

where

$$\Delta_L=\begin{pmatrix}\mathbf{1}_2 & -\mathscr{M} & 0\\ 0 & \bar{U} & 0\\ 0 & 0 & \mathbf{1}_2\end{pmatrix},\quad \Delta_R=\begin{pmatrix}\mathbf{1}_2 & 0 & 0\\ -\mathscr{M} & U & 0\\ 0 & 0 & \bar{d}\end{pmatrix}, \tag{2.30}$$

with

$$\bar{U}=\begin{pmatrix}-1 & 0\\ 0 & \Box\end{pmatrix},\quad U=\begin{pmatrix}\Box & 0\\ 0 & -1\end{pmatrix}, \tag{2.31a}$$

$$\bar{d} = (i\not{\nabla} + \mathscr{N})\mathbb{1}_2 . \tag{2.31b}$$

We then find

$$\Delta_W = \begin{pmatrix} \Delta_z' & 0 & \bar{\mathscr{F}}\bar{d} \\ 0 & \Box & 0 \\ \mathscr{F} & 0 & d\bar{d} \end{pmatrix}, \tag{2.32}$$

where

$$\Delta_z' = \Delta_z + \mathscr{M}^2 , \tag{2.33}$$

so that Δ_W is manifestly second order.

From (2.29) and (2.30),

$$\ln \operatorname{sdet} \Delta_V = \ln \operatorname{sdet} \Delta_W - 2 \ln \det \Box + \ln \det \bar{d} . \tag{2.34}$$

If neither d nor $\bar{d}$ have zero modes then neglecting finite anomaly contributions

$$\ln \det \bar{d} = \tfrac{1}{2} \ln \det d\bar{d} = \tfrac{1}{2} \ln \det \bar{d}d . \tag{2.35}$$

The operators Δ_W, $\Box$, and $\Delta_\chi = d\bar{d}$ are all of the form

$$\Delta = D_\mu D^\mu + Y^\Delta , \quad D_\mu = \nabla_\mu + X_\mu^\Delta . \tag{2.36}$$

For such an operator, the Schwinger–De Witt kernel[14,23,24] $\mathscr{G}_\Delta(x,x';s)$ is defined by

$$i\frac{\partial \mathscr{G}_\Delta}{\partial s} = \Delta \mathscr{G}_\Delta , \quad \mathscr{G}_\Delta(x,x';0) = \delta^d(x,x') . \tag{2.37}$$

The kernel has an asymptotic expansion as $s \downarrow 0$ of the form $\mathscr{G}_\Delta(x,x';s)$

$$\underset{s\downarrow 0}{\sim} [i/(4\pi i s)^{d/2}] e^{-i\sigma(x,x')/2s} \Delta_{\mathrm{VM}}^{1/2}(x,x') \times \sum_{n=0}^{\infty} a_n^\Delta(x,x')(is)^n , \tag{2.38}$$

where $\sigma(x,x')$ is half the square of the geodesic distance between x' and x, and Δ_{VM} is the Van Vleck–Morette determinant.[25] As is well known, we have

$$\ln \det \Delta = -\int_0^\infty \frac{ds}{s} \int dv_x \operatorname{tr} \mathscr{G}_\Delta(x,x;s) \tag{2.39}$$

and so, after substituting (2.38) in (2.39), we find

$$(\ln \det \Delta)^{\mathrm{pole}} = -i\frac{2}{\epsilon}\frac{\mu^{-\epsilon}}{16\pi^2}\int dv_x \operatorname{tr} a_2^\Delta(x,x) , \tag{2.40}$$

with a similar result for the superdeterminant obtained by replacing the trace with the supertrace. From (A2d) in the Appendix,

$$a_2^\Delta(x,x) = \tfrac{1}{12} G^\Delta_{\alpha\beta} G^{\Delta\alpha\beta} + \tfrac{1}{2}(2a^2\mathbb{1}^\Delta + Y^\Delta)^2 + \tfrac{1}{6}\mathscr{D}^2 Y^\Delta - \tfrac{1}{15} a^4 \mathbb{1}^\Delta , \tag{2.41}$$

where $\mathbb{1}^\Delta$ is the unit matrix for the space in which Δ acts, and

$$G_{\alpha\beta} = [\nabla_\alpha, \nabla_\beta] , \quad \mathscr{D}_\mu Y = \nabla_\mu Y + [X_\mu, Y] . \tag{2.42}$$

We have for Δ_W and Δ_χ

$$Y^\chi = -3a^2\mathbb{1}_2 + \mathscr{N}^2 - i\not{\nabla}\mathscr{N} , \quad X_\mu^\chi = 0 ,$$
$$G_{\alpha\beta}^\chi = -\tfrac{1}{4} R_{\alpha\beta\rho\sigma}\gamma^\rho\gamma^\sigma , \tag{2.43}$$

$$Y^W = \begin{pmatrix} -(\mathscr{V} - \mathscr{M}^2) & 0 & \bar{\mathscr{G}} \\ 0 & 0 & 0 \\ \mathscr{F} & 0 & Y^\chi \end{pmatrix}, \tag{2.44a}$$

$$X_\mu^W = \begin{pmatrix} 0 & 0 & \tfrac{1}{2} i \bar{\mathscr{F}}\gamma_\mu \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{2.44b}$$

$$G_{\alpha\beta}^W = \begin{pmatrix} 0 & 0 & \tfrac{1}{2} i \bar{\mathscr{F}}(\overleftarrow{\nabla}_\alpha\gamma_\beta - \overleftarrow{\nabla}_\beta\gamma_\alpha) \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{2.44c}$$

where, in (2.44a),

$$\bar{\mathscr{G}} = \bar{\mathscr{F}}\mathscr{N} - \tfrac{1}{2} i \bar{\mathscr{F}}\overleftarrow{\not{\nabla}} . \tag{2.45}$$

Since

$$-2a^2\mathbb{1}_2 + \mathscr{V} - \mathscr{M}^2 = \begin{pmatrix} -\bar{M}M & (\bar{K} + a\bar{M}) \\ (K + aM) & -M\bar{M} \end{pmatrix}, \tag{2.46a}$$

$$-2a^2\mathbb{1}_2 - Y^\chi = \begin{pmatrix} -\bar{M}M + a^2 & i\not{\nabla}\bar{M} \\ i\not{\nabla}M & -M\bar{M} + a^2 \end{pmatrix}, \tag{2.46b}$$

we find, from (2.34), (2.35), (2.40), (2.41), and (2.43)–(2.46),

$$\tfrac{1}{2} i(\ln \operatorname{sdet} \Delta_V)^{\mathrm{pole}} = \frac{\mu^{-\epsilon}}{16\pi^2\epsilon}\int dv_x \operatorname{tr}\{\nabla_\mu \bar{M}\nabla^\mu M + i\bar{\Lambda}\not{\nabla}\Lambda + (\bar{K} + a\bar{M})(K + aM) + 2a^2\bar{M}M - \tfrac{1}{2}a^4 S\} . \tag{2.47}$$

From (2.20) and (2.24),

$$M_{ab} = \mu^{(1/2)\epsilon}\lambda_{abc}z^c + \kappa_{ab} , \quad \bar{M}^{ab} = \mu^{(1/2)\epsilon}\bar{\lambda}^{abc}z_c^\dagger + \bar{\kappa}^{ab} , \tag{2.48}$$

and therefore, from (2.25c) and (2.48),

$$\operatorname{tr}[(\bar{K} + a\bar{M})(K + aM)] = \mu^\epsilon[F^\dagger SF + a(z^\dagger SF + F^\dagger Sz) + a^2 z^\dagger Sz] + \mu^{\epsilon/2}[a(T^\dagger F + F^\dagger T) + 2a^2(T^\dagger z + z^\dagger T)] + a^2\kappa_{ab}\bar{\kappa}^{ab} , \tag{2.49a}$$

$$\operatorname{tr}\bar{M}M = \mu^\epsilon z^\dagger Sz + \mu^{\epsilon/2}(T^\dagger z + z^\dagger T) + \kappa_{ab}\bar{\kappa}^{ab} , \tag{2.49b}$$

$$\operatorname{tr}(\nabla_\mu \bar{M}\nabla^\mu M) = \mu^\epsilon \nabla_\mu z^\dagger S\nabla^\mu z , \tag{2.49c}$$

$$\bar{\Lambda}\not{\nabla}\Lambda = \mu^\epsilon \bar{\chi} S\not{\nabla}\chi , \tag{2.49d}$$

where

$$S^a{}_b = \bar{\lambda}^{acd}\lambda_{cdb} , \tag{2.50a}$$

$$T^a = \bar{\lambda}^{abc}\kappa_{bc} . \tag{2.50b}$$

So, inserting (2.49) into (2.47),

$$\tfrac{1}{2} i(\ln \operatorname{sdet} \Delta_V)^{\mathrm{pole}} = \frac{1}{16\pi^2\epsilon}\int dv_x \{\nabla_\mu z^\dagger S\nabla^\mu z + i\bar{\chi}S\not{\nabla}\chi + F^\dagger SF + a(z^\dagger SF + F^\dagger Sz) + 3a^2 z^\dagger Sz + \mu^{-\epsilon/2}[a(T^\dagger F + F^\dagger T) + 3a^2(T^\dagger z + z^\dagger T)] + \mu^{-\epsilon}[3a^2\kappa_{ab}\bar{\kappa}^{ab} - \tfrac{1}{2}a^4 \operatorname{tr} S]\} . \tag{2.51}$$

Inserting into (2.26), we find that $W^{(1)}$ may be rendered finite by taking in $S^{(1)}$

$$Z_S^{(1)} = Z_A^{(1)} = Z_F^{(1)} = Z_{SA}^{(1)} = Z_Q^{(1)} = -(1/16\pi^2\epsilon)S \tag{2.52}$$

and

$$w^{(1)} = (-a/16\pi^2\epsilon)\{\mu^{\epsilon/2}T^\dagger z + \kappa_{ab}\bar{\kappa}^{ab} - \tfrac{1}{6}a^2 \operatorname{tr} S\}. \tag{2.53}$$

Hence the divergences preserve supersymmetry at one-loop order. However, the necessity for adding a counterterm to w, first recognized by Düsedau and Freedman,[9] vitiates the nonrenormalization theorem,[13] which is valid on flat space-times. Closely similar behavior is exhibited at two-loop order, as we shall show in the next section.

The results in (2.52) are consistent with those obtained by Bellucci and Gonzalez[8] and also by Düsedau and Freedman.[9] Bellucci and Gonzalez[10] also calculated the one-point functions for the scalar and auxiliary fields. In our formalism the one-loop one-point functions for z and F are given by $(\partial W^{(1)}/\partial z)|_{z=0,F=0,\chi=0}$ and $(\partial W^{(1)}/\partial F)|_{z=0,F=0,\chi=0}$ and hence their divergences arise from the terms linear in z and F in (2.51). These terms correspond precisely to the divergences Bellucci and Gonzalez[10] found for their one-point functions.

Düsedau and Freedman[9] calculated the one-point function for the scalar field after eliminating the auxiliary field by using its equation of motion

$$F^a = -\mu^{-\epsilon}\bar{w}^a - az^a. \tag{2.54}$$

After using (2.54) in (2.51), the linear terms assume the form

$$\frac{1}{16\pi^2\epsilon}\int dv_x\{a[T^\dagger(2az - \kappa z^\dagger) + (2az^\dagger - z\bar{\kappa})T]\mu^{-\epsilon/2} - \tfrac{1}{2}a(T_a^\dagger\bar{\lambda}^{abc}z_b^\dagger z_c^\dagger + T^a\lambda_{abc}z^b z^c) - a(T_a\bar{\nu}^a + T^a\nu_a)\mu^{-\epsilon}\}. \tag{2.55}$$

The linear term in z then yields a divergence corresponding to that found by Düsedau and Freedman for the one-point function of the scalar field. They inserted a counterterm analogous to (2.53) before calculating the two-point functions and hence eliminated the divergence from the quadratic term in (2.55).

III. TWO-LOOP CALCULATION

In this section we shall calculate the two-loop counterterms for the quantized Wess–Zumino model on $(AdS)_4$. We shall demonstrate that they have the same form as the one-loop counterterms in (2.51). We rely heavily on a general technique devised earlier[16] for the evaluation of two-loop divergences. The reader is referred to Ref. 16 for a detailed description of the method and a comprehensive list of references. We shall confine ourselves here to a brief account of the salient features of the procedure.

In the context of the background field method[14,15] the two-loop vacuum functional $W^{(2)}$ is expressed as a sum of vacuum Feynman graphs constructed using propagators derived from the Green's function G_V for Δ_V in (2.21), defined by

$$\Delta_V G_V(x,x') = -\delta^d(x,x'). \tag{3.1}$$

As we remarked in Sec. II, Δ_V is not of an appropriate form for application of techniques based on the Schwinger–De Witt kernel.[14,23,24] We focus attention instead on the operator Δ_W defined in (2.29), whose Green's function satisfies

$$\Delta_W G_W(x,x') = -\delta^d(x,x'). \tag{3.2}$$

By virtue of (2.29), G_V and G_W are related by

$$G_V = \Delta_R G_W \Delta_L. \tag{3.3}$$

The Green's function for an operator Δ of the form (2.36) can be written, using (2.37), as

$$G_\Delta(x,x') = -i\int_0^\infty ds\, \mathcal{G}_\Delta(x,x';s), \tag{3.4}$$

and has an expansion corresponding to (2.38),

$$G_\Delta(x,x') = -i\{G_0(x,x')a_0^\Delta(x,x') + R_1(x,x')a_1^\Delta(x,x') + R_2(x,x')a_2^\Delta(x,x')\} + H^\Delta(x,x'), \tag{3.5}$$

where

$$G_0(x,x') = \frac{\Gamma(\frac{1}{2}d-1)}{4\pi^{(1/2)d}}\frac{\Delta_{VM}^{1/2}}{(-2\sigma)^{(1/2)d-1}}, \tag{3.6a}$$

$$R_n = \frac{\Delta_{VM}^{1/2}}{4^{n+1}}\left\{\frac{1}{\pi^{(1/2)d}}\Gamma\left(\frac{1}{2}d-1-n\right)(-2\sigma)^{n+1-(1/2)d} - \frac{(-1)^n}{\pi^2(n-1)!}\frac{2}{\epsilon}(-2\sigma)^{n-1}\mu^{-\epsilon}\right\}. \tag{3.6b}$$

The first three terms on the right-hand side of (3.5) account for all local divergences of a renormalizable theory in four dimensions. The remainder term H^Δ is finite as $\epsilon\downarrow 0$ and nonsingular as $x\sim x'$ with up to two derivatives acting on it. When the expansion (3.5) is substituted into the expression for a two-loop Feynman graph, divergences arise from products of two or three functions of the type G_0 or R_n in (3.6). All such divergences are tabulated in Ref. 16. They take the form of a δ-function with up to four derivatives acting on it, multiplying poles in ϵ. After performing a spatial integration we are required to evaluate the coincidence limits of products of a_n^Δ's with various derivatives acting on

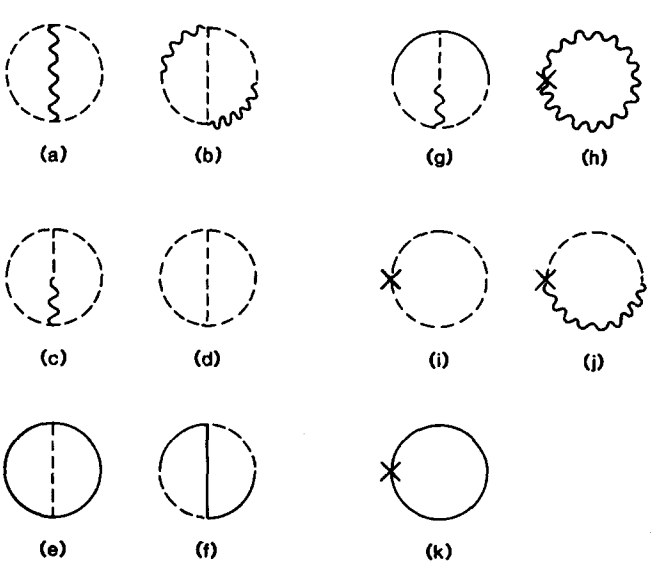

FIG. 1. Two-loop diagrams.

them. Some useful identities are given in the Appendix.

The Feynman graphs are constructed with vertices furnished by the interaction term S_I in (2.21). Explicitly this has the form

$$S_I = \frac{\mu^{(1/2)\epsilon}}{2}\int dv_x \{\lambda_{abc}\, y^a y^b f^c + \bar{\lambda}^{abc} y_a^\dagger\, y_b^\dagger f_c^\dagger - \lambda_{abc}\, y^a \bar{\eta}'^b \eta^c - \bar{\lambda}^{abc} y_a^\dagger \bar{\eta}_b \eta'_c + a\lambda_{abc}\, y^a y^b y^c + a\bar{\lambda}^{abc} y_a^\dagger\, y_b^\dagger\, y_c^\dagger\}\,. \tag{3.7}$$

As far as divergences are concerned, we need only consider one-particle-irreducible (1PI) diagrams contributing to $W^{(2)}$ (in other words precisely those diagrams contributing to the effective action).

Writing

$$G_V = \begin{pmatrix} g^S & g^{SA} & g^{SF} \\ g^{AS} & g^A & g^{AF} \\ g^{FS} & g^{FA} & g^F \end{pmatrix}, \tag{3.8}$$

we have the following amplitudes for the diagrams giving divergent contributions to $W^{(2)}$ shown in Fig. 1 (with scalar, fermion, auxiliary indices represented by dashed, unbroken, and wavy lines, respectively):

$$W^{(2)}_{\rm 1PI}[z,z^\dagger,F,F^\dagger,\chi,\bar{\chi}]_a = \frac{\mu^\epsilon}{2}\int dv_x\, dv_{x'}\lambda_{abc}\bar{\lambda}^{def} g^{Sa}{}_d g^{Sb}{}_e g^{Ac}{}_f\,, \tag{3.9a}$$

$$W^{(2)}_{\rm 1PI}[z,z^\dagger,F,F^\dagger,\chi,\bar{\chi}]_b = \mu^\epsilon\int dv_x\, dv_{x'}\left\{\lambda_{abc}\bar{\lambda}^{def} g^{Sa}{}_d g^{ASb}{}_e g^{SAc}{}_f + \frac{1}{2}\lambda_{abc}\lambda_{def}\, g^{Bad} g^{ASbe} g^{SAcf} + \frac{1}{2}\bar{\lambda}^{abc}\bar{\lambda}^{def} g^S{}_{ad}\, g^{AS}{}_{be}\, g^{SA}{}_{cf}\right\}, \tag{3.9b}$$

$$W^{(2)}_{\rm 1PI}[z,z^\dagger,F,F^\dagger,\chi,\bar{\chi}]_c = \frac{3}{2}\mu^\epsilon a\int dv_x\, dv_{x'}\lambda_{abc}\bar{\lambda}^{def} g^{Sa}{}_d g^{Sb}{}_e (g^{ASc}{}_f + g^{SAc}{}_f)\,, \tag{3.9c}$$

$$W^{(2)}_{\rm 1PI}[z,z^\dagger,F,F^\dagger,\chi,\bar{\chi}]_d = \frac{3}{2}\mu^\epsilon a^2\int dv_x\, dv_{x'}\lambda_{abc}\bar{\lambda}^{def} g^{Sa}{}_d\, g^{Sb}{}_e\, g^{Sc}{}_f\,, \tag{3.9d}$$

$$\begin{aligned} W^{(2)}_{\rm 1PI}[z,z^\dagger,F,F^\dagger,\chi,\bar{\chi}]_e = -\frac{\mu^\epsilon}{2}\int dv_x\, dv_{x'}\{&\mathrm{tr}[\lambda_{abc}\, g^{Fc}{}_d(x,x')\bar{\lambda}^{def} g^F{}_f{}^a(x',x)]g^{Sb}{}_e(x,x') \\ &+ \tfrac{1}{2}\,\mathrm{tr}[\lambda_{abc}\, g^{Fcd}(x,x')\lambda_{def}\, g^{Ffa}(x',x)]g^{Sbe}(x,x') \\ &+ \tfrac{1}{2}\,\mathrm{tr}[\bar{\lambda}^{abc} g^F{}_{cd}(x,x')\bar{\lambda}^{def} g^F{}_{fa}(x',x)]g^S{}_{be}(x,x')\}\,, \end{aligned} \tag{3.9e}$$

$$W^{(2)}_{\rm 1PI}[z,z^\dagger,F,F^\dagger,\chi,\bar{\chi}]_f = \mu^\epsilon\int dv_x\, dv_{x'}\, g^{SF}{}_a{}^b(x',x)\lambda_{bcd}\, g^{Fd}{}_e(x,x')\bar{\lambda}^{eaf} g^{FS}{}_f{}^c(x',x)\,, \tag{3.9f}$$

$$\begin{aligned} &W^{(2)}_{\rm 1PI}[z,z^\dagger,F,F^\dagger,\chi,\bar{\chi}]_g \\ &= -\frac{\mu^\epsilon}{2}\int dv_x\, dv_{x'}\{g^{SFa}{}_b(x',x)\bar{\lambda}^{bcd} g^{SA}{}_d{}^e(x,x')\lambda_{eaf}\, g^{FS}{}_c{}^f(x,x') + g^{SF}{}_{ab}(x',x)\bar{\lambda}^{bcd} g^{SA}{}_{de}(x,x')\bar{\lambda}^{eaf} g^{FS}{}_{cf}(x,x') \\ &\quad + g^{SFab}(x',x)\lambda_{bcd}\, g^{SAde}(x,x')\lambda_{eaf}\, g^{FScf}(x,x') + g^{SF}{}_a{}^b(x',x)\lambda_{bcd}\, g^{SAd}{}_e(x,x')\bar{\lambda}^{eaf} g^{FSc}{}_f(x,x')\}\,, \end{aligned} \tag{3.9g}$$

$$W^{(2)}_{\rm 1PI}[z,z^\dagger,F,F^\dagger,\chi,\bar{\chi}]_h = -\frac{1}{2}\frac{i}{16\pi^2\epsilon}\int dv_x\,\mathrm{tr}(\bar{S}g^A)_{\rm diag}\,, \tag{3.9h}$$

$$W^{(2)}_{\rm 1PI}[z,z^\dagger,F,F^\dagger,\chi,\bar{\chi}]_i = -\frac{1}{2}\frac{i}{16\pi^2\epsilon}\int dv_x\{3a^2\,\mathrm{tr}(\bar{S}g^S)_{\rm diag} - \mathrm{tr}(\bar{S}\Box g^S)_{\rm diag}\}\,, \tag{3.9i}$$

$$W^{(2)}_{\rm 1PI}[z,z^\dagger,F,F^\dagger,\chi,\bar{\chi}]_j = -\frac{1}{2}\frac{ia}{16\pi^2\epsilon}\int dv_x\,\mathrm{tr}(\bar{S}g^{AS} + \bar{S}g^{SA})_{\rm diag}\,, \tag{3.9j}$$

$$W^{(2)}_{\rm 1PI}[z,z^\dagger,F,F^\dagger,\chi,\bar{\chi}]_k = -\frac{1}{2}\frac{1}{16\pi^2\epsilon}\int dv_x\,\mathrm{tr}(\bar{S}\not{\partial}g^F)_{\rm diag}\,. \tag{3.9k}$$

The diagrams (3.9a)–(3.9g) are the genuine two-loop diagrams generated by the interactions in (3.7), while the diagrams (3.9h)–(3.9k) represent counterterm diagrams arising from substituting the one-loop results in (2.52) and (2.53) into Δ_V^B in (2.2). In (3.9a)–(3.9g) we have suppressed the arguments of the Green's functions when they occur in the usual order, x,x'. In (3.9h)–(3.9k) the subscript diag indicates the coincidence limit as $x'\to x$, and

$$\bar{S} = \begin{pmatrix} S & 0 \\ 0 & S \end{pmatrix}.$$

We may now use (3.3) to express the amplitude for each diagram in terms of G_W and then apply the standard technique adumbrated earlier to extract the divergences. Writing

$$G_W = \begin{pmatrix} G^S & G^{SA} & G^{SF} \\ G^{AS} & G^A & G^{AF} \\ G^{FS} & G^{FA} & G^F \end{pmatrix}, \tag{3.10}$$

we have, from (3.3), (3.8), and (2.30),

$$g^S = G^S,\quad g^{AS} = -\mathscr{M}G^S + UG^{AS},\quad g^{SA} = -G^S\mathscr{M} + G^{SA}\bar{U},\quad g^A = \mathscr{M}G^S\mathscr{M} - \mathscr{M}G^{SA}\bar{U} - UG^{SA}\mathscr{M} + UG^A\bar{U},$$
$$g^{SF} = G^{SF},\quad g^{FS} = \bar{d}G^{FS},\quad g^{FA} = -\mathscr{M}G^{FS} + \bar{d}G^{FA}\bar{U},\quad g^{AF} = -\mathscr{M}G^{SF} + UG^{AF},\quad g^F = \bar{d}G^F. \tag{3.11}$$

The AS and SA components of every heat kernel coefficient for Δ_W are zero and so we may disregard G^{AS} and G^{SA}.

In the case of the diagrams that do not arise from interactions involving auxiliary fields, namely (3.9d)–(3.9f), (3.9i), and (3.9k), we can obtain the divergences from general results calculated previously.[26,27] In the case of the remaining diagrams we can compute the divergences *ab initio* fairly straightforwardly. For the genuine two-loop diagrams, after using (3.11) to express components of G_V in terms of those of G_W, we substitute the expansion (3.5) for G_W. We then use the results tabulated in Ref. 16 to obtain the divergent parts of products of two or three functions of the type G_0 or R_n, in the form of pole terms multiplying derivatives of δ-functions. We may then integrate over x' and use the results in the Appendix to evaluate the coincidence limits of the various heat kernel coefficients a_n and their derivatives that occur. We shall exemplify the procedure by examining the contribution from (3.9a) in some detail. From (3.11) we may rewrite (3.9a) in the form

$$W^{(2)}_{1PI}[z,z^\dagger,F,F^\dagger,\chi,\bar{\chi}]_a = I_1 + I_2 + I_3 + I_4, \tag{3.12}$$

where

$$I_1 = \frac{\mu^\epsilon}{2}\int dv_x\, dv_{x'}\, \lambda_{abc}\bar{\lambda}^{def}G^{Sa}{}_dG^{Sb}{}_e(\bar{M}^{cg}G^S{}_g{}^hM_{hf} + a^2G^{Sc}{}_f), \tag{3.13a}$$

$$I_2 = \frac{\mu^\epsilon}{2}a\int dv_x\, dv_{x'}\, \lambda_{abc}\bar{\lambda}^{def}G^{Sa}{}_dG^{Sb}{}_eG^{Sch}M_{hf}, \tag{3.13b}$$

$$I_3 = \frac{\mu^\epsilon}{2}a\int dv_x\, dv_{x'}\, \lambda_{abc}\bar{\lambda}^{def}G^{Sa}{}_dG^{Sb}{}_e\bar{M}^{cg}G^S{}_{gf}, \tag{3.13c}$$

$$I_4 = \frac{\mu^\epsilon}{2}\int dv_x\, dv_{x'}\, \lambda_{abc}\bar{\lambda}^{def}G^{Sa}{}_dG^{Sb}{}_e(-\Box G^A)^c{}_f. \tag{3.13d}$$

Let us consider I_1. We have, from (3.5),

$$I_1^{\text{pole}} = \frac{i\mu^\epsilon}{2}\int dv_x\, dv_{x'}\, \lambda_{abc}\bar{\lambda}^{def}\{G_0^2R_1[a_0^{Sa}{}_da_0^{Sb}{}_e(\bar{M}^{cg}a_1^S{}_g{}^hM_{hf} + a^2a_1^{Sc}{}_f) + 2a_1^{Sa}{}_da_0^{Sb}{}_e(\bar{M}^{cg}a_0^S{}_g{}^hM_{hf} + a^2a_0^{Sc}{}_f)]$$
$$+ G_0^3a_0^{Sa}{}_da_0^{Sb}{}_e(\bar{M}^{cg}a_0^S{}_g{}^hM_{hf} + a^2a_0^{Sc}{}_f)\}$$
$$-\frac{\mu^\epsilon}{2}\int dv_x\, dv_{x'}\lambda_{abc}\bar{\lambda}^{def}G_0^2\{a_0^{Sa}{}_da_0^{Sb}{}_e(\bar{M}^{cg}H^S{}_g{}^hM_{hf} + a^2H^{Sc}{}_f) + 2H^{Sa}{}_da_0^{Sb}{}_e(\bar{M}^{cg}a_0^S{}_g{}^hM_{hf} + a^2a_0^{Sc}{}_f)\}. \tag{3.14}$$

Referring to Ref. 16 and making allowances for the change from Euclidean to Lorentzian signature, we find

$$G_0{}^2R_1 \sim \frac{-i\mu^{-2\epsilon}}{(16\pi^2)^2}\left(\frac{2}{\epsilon^2} + \frac{1}{\epsilon}\right)\delta^d(x,x'), \tag{3.15a}$$

$$G_0{}^3 \sim \frac{i\mu^{-2\epsilon}}{(16\pi^2)^2}\frac{1}{\epsilon}\frac{1}{2}(\Box + 2a^2)\delta^d(x,x'), \tag{3.15b}$$

$$G_0{}^2 \sim \frac{-i\mu^{-\epsilon}}{16\pi^2}\frac{2}{\epsilon}\delta^d(x,x'), \tag{3.15c}$$

and hence, using the following results obtained by substituting (2.44a) into (A2) in the Appendix,

$$(a_1^{Sa}{}_b)_{\text{diag}} = -(\bar{M}M)^a{}_b,\quad (a_0^{Sa}{}_b)_{\text{diag}} = \delta^a{}_b, \tag{3.16}$$

we have, after substituting (3.15) into (3.14) and integrating by parts,

$$I_1^{\text{pole}} = -\frac{\mu^{-\epsilon}}{(16\pi^2)^2}\int dv_x\left\{\left\{\frac{2}{\epsilon^2} + \frac{1}{\epsilon}\right\}\left[\lambda_{abc}(\bar{M}M)^b{}_e\bar{\lambda}^{aef}(\bar{M}M)^c{}_f + \frac{1}{2}\operatorname{tr}(S\bar{M}M\bar{M}M) + \frac{3}{2}a^2\operatorname{tr}(S\bar{M}M)\right] + \frac{1}{2}\frac{1}{\epsilon}a^4\operatorname{tr}S\right.$$
$$\left. - \frac{1}{4}\frac{1}{\epsilon}\operatorname{tr}[\nabla_\mu\bar{M}S\nabla^\mu M] + \frac{1}{2}\frac{1}{\epsilon}a^2\operatorname{tr}(S\bar{M}M)\right\} + \frac{i}{16\pi^2}\frac{1}{\epsilon}\int dv_x\{\operatorname{tr}(S\bar{M}H^SM) + 2\lambda_{abc}\bar{\lambda}^{dbe}(\bar{M}M)^c{}_fH^{Sa}{}_e$$
$$+ 3a^2\operatorname{tr}(SH^S)\}_{\text{diag}}. \tag{3.17}$$

For I_2, we have

$$I_2^{\text{pole}} = \frac{ia\mu^\epsilon}{2}\int dv_x\, dv_{x'}\lambda_{abc}\bar{\lambda}^{def}\{G_0^2R_1[a_0^{Sa}{}_da_0^{Sb}{}_ea_1^{Sch}M_{hf} + 2a_1^{Sa}{}_da_0^{Sb}{}_ea_0^{Sch}M_{hf}] + G_0^3a_0^{Sa}{}_da_0^{Sb}{}_ea_0^{Sch}M_{hf}\}$$
$$-\frac{a\mu^\epsilon}{2}\int dv_x\, dv_{x'}G_0^2\{a_0^{Sa}{}_da_0^{Sb}{}_eH^{Sch}M_{hf} + 2H^{Sa}{}_da_0^{Sb}{}_ea_0^{Sch}M_{hf}\}. \tag{3.18}$$

Using (3.15) once more, but now with the coincidence limits

$$(a_1{}^{Sab})_{\rm diag} = (\bar{K} + a\bar{M})^{ab}\,, \quad (a_0{}^{Sab})_{\rm diag} = 0\,, \tag{3.19}$$

we obtain

$$I_2^{\rm pole} = \frac{1}{2}\, a\, \frac{\mu^{-\epsilon}}{(16\pi^2)^2}\left(\frac{2}{\epsilon^2} + \frac{1}{\epsilon}\right)\int dv_x\ {\rm tr}[S(\bar{K} + a\bar{M})M] + ia\,\frac{1}{16\pi^2}\,\frac{1}{\epsilon}\int dv_x\ {\rm tr}(SH^S M)_{\rm diag}\,. \tag{3.20}$$

Similarly,

$$I_3^{\rm pole} = \frac{1}{2}\, a\, \frac{\mu^{-\epsilon}}{(16\pi^2)^2}\left(\frac{2}{\epsilon^2} + \frac{1}{\epsilon}\right)\int dv_x\ {\rm tr}[S\bar{M}(K + aM)] + ia\,\frac{1}{16\pi^2}\,\frac{1}{\epsilon}\int dv_x\ {\rm tr}(S\bar{M}H^S)_{\rm diag}\,. \tag{3.21}$$

Finally,

$$\begin{aligned} I_4^{\rm pole} = \frac{i\mu^{\epsilon}}{2}\int dv_x\, dv_{x'}\lambda_{abc}\bar{\lambda}^{def}\{&G_0{}^2(-\Box G_0)a_0{}^{Sa}{}_d a_0{}^{Sb}{}_e a_0{}^{Ac}{}_f + 2G_0R_1(-\Box G_0)a_0{}^{Sa}{}_d a_1{}^{Sb}{}_e a_0{}^{Ac}{}_f \\ &+ G_0{}^2(-\Box R_1)a_0{}^{Sa}{}_d a_0{}^{Sb}{}_e a_1{}^{Ac}{}_f - G_0{}^2R_1 a_0{}^{Sa}{}_d a_0{}^{Sb}{}_e(\Box a_1{}^A)^c{}_f - 2G_0{}^2\partial_\mu R_1 a_0{}^{Sa}{}_d a_0{}^{Sb}{}_e(\partial^\mu a_1{}^A)^c{}_f \\ &+ 2G_0R_1(-\Box R_1)a_0{}^{Sa}{}_d a_1{}^{Sb}{}_e a_1{}^{Ac}{}_f + R_1{}^2(-\Box G_0)a_1{}^{Sa}{}_d a_1{}^{Sb}{}_e a_0{}^{Ac}{}_f \\ &+ G_0{}^2(-\Box R_2)a_0{}^{Sa}{}_d a_0{}^{Sb}{}_e a_2{}^{Ac}{}_f + G_0(-\Box G_0)R_2 a_2{}^{Sa}{}_d a_0{}^{Sb}{}_e a_0{}^{Ac}{}_f\} - \frac{\mu^{\epsilon}}{2}\int dv_x\,\lambda_{abc}\bar{\lambda}^{def}\{G_0{}^2 a_0^{Sa}{}_d a_0^{Sb}{}_e(-\Box H^A)^c{}_f \\ &+ 2(-\Box G_0)R_1 H^{Sa}{}_d a_1{}^{Sb}{}_e a_0{}^{Ac}{}_f + 2G_0(-\Box R_1)H^{Sa}{}_d a_0{}^{Sb}{}_e a_1{}^{Ac}{}_f + G_0(-\Box G_0)H^{Sa}{}_d a_0{}^{Sb}{}_e a_0{}^{Ac}{}_f\}\,. \end{aligned} \tag{3.22}$$

We find, consulting Ref. 16 again and once more taking account of the change in space-time signature,

$$G_0{}^2(-\Box G_0) \sim \frac{-i\mu^{-2\epsilon}}{(16\pi^2)^2}\,\frac{1}{\epsilon}\,\frac{9}{5}\,a^4\delta^d(x,x')\,, \tag{3.23a}$$

$$G_0R_1(-\Box G_0) \sim \frac{i\mu^{-2\epsilon}}{(16\pi^2)^2}\,4\left(\frac{1}{\epsilon^2} + \frac{1}{2}\,\frac{1}{\epsilon}\right)a^2\delta^d(x,x')\,, \tag{3.23b}$$

$$G_0{}^2(-\Box R_1) \sim \frac{-i\mu^{-2\epsilon}}{(16\pi^2)^2}\left\{\frac{1}{2}\,\frac{1}{\epsilon}\,\Box - 4\left(\frac{1}{\epsilon^2} + \frac{1}{4}\,\frac{1}{\epsilon}\right)a^2\right\}\delta^d(x,x')\,, \tag{3.23c}$$

$$G_0{}^2\,\partial_\mu R_1 \sim \frac{-i\mu^{-2\epsilon}}{(16\pi^2)^2}\,\frac{1}{\epsilon}\,\frac{1}{2}\,\partial_\mu\delta^d(x,x')\,, \tag{3.23d}$$

$$G_0R_1(-\Box R_1) \sim \frac{i\mu^{-2\epsilon}}{(16\pi^2)^2}\,2\left(\frac{1}{\epsilon^2} + \frac{1}{2}\,\frac{1}{\epsilon}\right)\delta^d(x,x')\,, \tag{3.23e}$$

$$R_1{}^2(-\Box G_0) \sim 4[i\mu^{-2\epsilon}/(16\pi^2\epsilon)^2]\delta^d(x,x')\,, \tag{3.23f}$$

$$G_0{}^2(-\Box R_2) \sim 4[i\mu^{-2\epsilon}/(16\pi^2\epsilon)^2]\delta^d(x,x')\,, \tag{3.23g}$$

$$G_0(-\Box G_0)R_2 \sim 0\,, \tag{3.23h}$$

$$G_0(-\Box G_0) \sim 4(i\mu^{-\epsilon}/16\pi^2)(1/\epsilon)a^2\delta^d(x,x')\,, \tag{3.23i}$$

$$G_0(-\Box R_1) \sim 2\,\frac{i\mu^{-\epsilon}}{16\pi^2}\,\frac{1}{\epsilon}\,\delta^d(x,x')\,, \tag{3.23j}$$

$$R_1(-\Box G_0) \sim 2\,\frac{i\mu^{-\epsilon}}{16\pi^2}\,\frac{1}{\epsilon}\,\delta^d(x,x')\,. \tag{3.23k}$$

Using (2.44) in conjunction with the general results in the Appendix we find

$$(a_1{}^{Aa}{}_b)_{\rm diag} = -2a^2\delta^a{}_b\,, \tag{3.24a}$$

$$(\Box a_1{}^{Aa}{}_b)_{\rm diag} = \tfrac{2}{15}\,a^4\delta^a{}_b\,, \tag{3.24b}$$

$$(a_2{}^{Aa}{}_b)_{\rm diag} = \tfrac{29}{15}\,a^4\delta^a{}_b\,, \tag{3.24c}$$

and hence, substituting results from (3.15) and (3.23) into (3.22), integrating over x', and using (3.16) and (3.24), we obtain

$$\begin{aligned} I_4^{\rm pole} = &-\frac{\mu^{-\epsilon}}{(16\pi^2)^2}\int dv_x\left\{\frac{2}{\epsilon^2}\,\lambda_{abc}(\bar{M}M)^b{}_e\bar{\lambda}^{aef}(\bar{M}M)^c{}_f - \frac{29}{15}\,\frac{1}{\epsilon}\,a^4\,{\rm tr}\,S\right\} \\ &+ \frac{i}{16\pi^2}\,\frac{1}{\epsilon}\int dv_x\{2\lambda_{abc}\bar{\lambda}^{dbe}(\bar{M}M)^c{}_f H^{Sa}{}_e - {\rm tr}(S\Box H^A)\}_{\rm diag}\,. \end{aligned} \tag{3.25}$$

Adding (3.17), (3.20), (3.21), and (3.25), we find

$$W^{(2)}_{1PI}[z,z^\dagger,F,F^\dagger,\chi,\bar\chi]^{\rm pole}_a$$
$$= -\frac{\mu^{-\epsilon}}{(16\pi^2)^2}\int dv_x\left\{\frac{1}{2}\left(\frac{2}{\epsilon^2}+\frac{1}{\epsilon}\right)[\mathrm{tr}(S\bar M M\bar M M)+3a^2\,\mathrm{tr}(S\bar M M)-a\,\mathrm{tr}[S(\bar K+a\bar M)M+S\bar M(K+aM)]]\right.$$
$$\left.+\left(\frac{4}{\epsilon^2}+\frac{1}{\epsilon}\right)\lambda_{abc}(\bar M M)^b{}_e\bar\lambda^{aef}(\bar M M)^c{}_f-\frac{1}{4}\frac{1}{\epsilon}\mathrm{tr}[\nabla_\mu\bar M S\nabla^\mu M]-\frac{43}{30}\frac{1}{\epsilon}a^4\,\mathrm{tr}\,S+\frac{1}{2}\frac{1}{\epsilon}a^2\,\mathrm{tr}(S\bar M M)\right\}$$
$$+\frac{i}{16\pi^2}\frac{1}{\epsilon}\int dv_x\{\mathrm{tr}(S\bar M H^S M)+4\lambda_{abc}\bar\lambda^{dbe}(\bar M M)^c{}_f H^{Sa}{}_e+3a^2\,\mathrm{tr}(SH^S)$$
$$+a\,\mathrm{tr}(S\bar M H^S)+a\,\mathrm{tr}(SH^S M)-\mathrm{tr}(S\Box H^A)\}_{\rm diag}\,. \tag{3.26}$$

The remaining genuine two-loop diagrams involving auxiliary fields, namely (3.9a), (3.9b), and (3.9g), can be treated in a similar fashion. We obtain divergent contributions as follows:

$$W^{(2)}_{1PI}[z,z^\dagger,F,F^\dagger,\chi,\bar\chi]^{\rm pole}_b$$
$$=\frac{\mu^{-\epsilon}}{(16\pi^2)^2}\int dv_x\left\{-3a^2\left(\frac{2}{\epsilon^2}+\frac{1}{\epsilon}\right)\mathrm{tr}(S\bar M M)+\left(\frac{2}{\epsilon^2}+\frac{1}{\epsilon}\right)a\,\mathrm{tr}\,S\,[\bar M(K+aM)+(\bar K+a\bar M)M]-\frac{1}{\epsilon}a^4\,\mathrm{tr}\,S\right.$$
$$\left.+\frac{1}{2}\left(\frac{2}{\epsilon^2}+\frac{1}{\epsilon}\right)[\lambda_{abc}\lambda_{def}\bar M^{be}\bar M^{cf}(\bar K+a\bar M)^{ad}+\bar\lambda^{abc}\bar\lambda^{def}M_{be}M_{cf}(K+aM)_{ad}]\right\}$$
$$+\frac{i}{16\pi^2}\frac{1}{\epsilon}\int dv_x\{6a^2\,\mathrm{tr}(SH^S)+2a[\mathrm{tr}(S\bar M H^S)+\mathrm{tr}(SH^S M)]$$
$$+\lambda_{abc}\lambda_{def}\bar M^{ad}\bar M^{be}H^{Scf}+\bar\lambda^{abc}\bar\lambda^{def}M_{ad}M_{be}H^S{}_{cf}\}_{\rm diag}\,, \tag{3.27}$$

$$W^{(2)}_{1PI}[z,z^\dagger,F,F^\dagger,\chi,\bar\chi]^{\rm pole}_c$$
$$=\frac{3}{2}\frac{\mu^{-\epsilon}}{(16\pi^2)^2}\int dv_x\left\{6\left(\frac{2}{\epsilon^2}+\frac{1}{\epsilon}\right)a^2\,\mathrm{tr}(S\bar M M)-\left(\frac{2}{\epsilon^2}+\frac{1}{\epsilon}\right)a\,\mathrm{tr}\,S\,[\bar M(K+aM)+(\bar K+a\bar M)M]+\frac{2}{\epsilon}a^4\,\mathrm{tr}\,S\right\}$$
$$-3\frac{i}{16\pi^2}\frac{1}{\epsilon}\int dv_x\{6a^2\,\mathrm{tr}(SH^S)+a\,\mathrm{tr}\,S(\bar M H^S+H^S M)\}_{\rm diag}\,, \tag{3.28}$$

$$W^{(2)}_{1PI}[z,z^\dagger,F,F^\dagger,\chi,\bar\chi]^{\rm pole}_g=-\frac{1}{2}\frac{\mu^{-\epsilon}}{(16\pi^2)^2}\frac{1}{\epsilon}\int dv_x\{\bar\Lambda'_{ab}\bar\lambda^{bcd}M_{de}\bar\lambda^{eaf}\Lambda_{cf}+\bar\Lambda^{ab}\lambda_{bcd}\bar M^{de}\lambda_{eaf}\Lambda'^{cf}\}\,. \tag{3.29}$$

In obtaining (3.29) we have used the result

$$(\partial_\mu a_0{}^{SF})_{\rm diag}=-\tfrac{1}{2}i\overline{\mathcal{F}}\gamma_\mu\,, \tag{3.30}$$

which can be proved using (A1a), (2.36), and (2.44b).

We also need to consider the counterterm diagrams (3.9h) and (3.9j), which contain auxiliary fields. Using (3.11) once more, we decompose (3.9h) according to

$$W^{(2)}_{1PI}[z,z^\dagger,F,F^\dagger,\chi,\bar\chi]_h=J_1+J_2+J_3+J_4\,, \tag{3.31}$$

where

$$J_1=-\frac{i}{16\pi^2}\frac{1}{\epsilon}\int dv_x\,\mathrm{tr}[S(\bar M G^S M+a^2G^S)]_{\rm diag}\,, \tag{3.32a}$$

$$J_2=-\frac{ia}{16\pi^2}\frac{1}{\epsilon}\int dv_x\,\mathrm{tr}(SG^S M)_{\rm diag}\,, \tag{3.32b}$$

$$J_3=-\frac{ia}{16\pi^2}\frac{1}{\epsilon}\int dv_x\,\mathrm{tr}(S\bar M G^S)_{\rm diag}\,, \tag{3.32c}$$

$$J_4=\frac{i}{16\pi^2\epsilon}\int dv_x\,(\Box G^A)_{\rm diag}\,. \tag{3.32d}$$

Using (A3) together with (3.16), (3.19), and (3.24), we obtain

$$J_1^{\rm pole}=2\frac{\mu^{-\epsilon}}{(16\pi^2\epsilon)^2}\int dv_x\{\mathrm{tr}[S\bar M M\bar M M]+a^2\,\mathrm{tr}(S\bar M M)\}-\frac{i}{16\pi^2}\frac{1}{\epsilon}\int dv_x\,\mathrm{tr}[S(\bar M H^S M+a^2H^S)]_{\rm diag}\,, \tag{3.33a}$$

$$J_2^{\rm pole}=-2a\frac{\mu^{-\epsilon}}{(16\pi^2\epsilon)^2}\int dv_x\,\mathrm{tr}[S(\bar K+a\bar M)M]-\frac{ia}{16\pi^2}\frac{1}{\epsilon}\int dv_x\,\mathrm{tr}(SH^S M)_{\rm diag}\,, \tag{3.33b}$$

$$J_3^{\rm pole}=-2a\frac{\mu^{-\epsilon}}{(16\pi^2\epsilon)^2}\int dv_x\,\mathrm{tr}[S\bar M(K+aM)]-\frac{ia}{16\pi^2}\frac{1}{\epsilon}\int dv_x\,\mathrm{tr}(S\bar M H^S)_{\rm diag}\,, \tag{3.33c}$$

$$J_4^{\rm pole}=-\frac{\mu^{-\epsilon}}{(16\pi^2)^2}\frac{1}{\epsilon}\frac{29}{15}a^4\int dv_x\,\mathrm{tr}\,S+\frac{i}{16\pi^2}\frac{1}{\epsilon}\int dv_x\,(\Box H^A)_{\rm diag}\,, \tag{3.33d}$$

so that, adding (3.33a)–(3.33d),

$$W^{(2)}_{\rm 1PI}[z,z^\dagger,F,F^\dagger,\chi,\bar\chi]^{\rm pole}_h$$
$$= 2\frac{\mu^{-\epsilon}}{(16\pi^2\epsilon)^2}\int dv_x\left\{\mathrm{tr}(S\bar M M\bar M M)+a^2\,\mathrm{tr}(S\bar M M)-a\,\mathrm{tr}[S(\bar K+a\bar M)M]-a\,\mathrm{tr}[S\bar M(K+aM)]-\frac{29}{30}a^4\,\mathrm{tr}\,S\right\}$$
$$-\frac{1}{2}\frac{i}{16\pi^2}\frac{1}{\epsilon}\int dv_x\{\mathrm{tr}(S\bar M H^S M)+a[\mathrm{tr}(S\bar M H^S)+\mathrm{tr}(SH^S M)]-\mathrm{tr}(S\Box H^S)\}_{\rm diag}\,. \tag{3.34}$$

In a similar fashion we find

$$W^{(2)}_{\rm 1PI}[z,z^\dagger,F,F^\dagger,\chi,\bar\chi]^{\rm pole}_j$$
$$= 2\frac{\mu^{-\epsilon}}{(16\pi^2\epsilon)^2}\int dv_x\{a\,\mathrm{tr}[S(\bar K+a\bar M)M]+a\,\mathrm{tr}[S\bar M(K+aM)]-2a^2\,\mathrm{tr}(S\bar M M)\}$$
$$+\frac{1}{2}\frac{ia}{16\pi^2}\frac{1}{\epsilon}\int dv_x\{\mathrm{tr}(S\bar M H^S)+\mathrm{tr}(SH^S M)+a\,\mathrm{tr}(SH^S)\}_{\rm diag}\,. \tag{3.35}$$

We now turn to the diagrams that involve only fermions and scalars. The procedures for calculating the divergences of two-loop graphs such as these have been described in detail in Refs. 26 and 27 and so we shall confine ourselves here to setting down the results:

$$W^{(2)}_{\rm 1PI}[z,z^\dagger,F,F^\dagger,\chi,\bar\chi]^{\rm pole}_d=\frac{3}{2}\frac{\mu^{-\epsilon}}{(16\pi^2)^2}\int dv_x\left\{-3a^2\left(\frac{2}{\epsilon^2}+\frac{1}{\epsilon}\right)\mathrm{tr}(S\bar M M)-\frac{1}{\epsilon}a^4\,\mathrm{tr}\,S\right\}+9\frac{i}{16\pi^2}\frac{1}{\epsilon}a^2\int dv_x\,\mathrm{tr}(SH^S)_{\rm diag}\,, \tag{3.36}$$

$$W^{(2)}_{\rm 1PI}[z,z^\dagger,F,F^\dagger,\chi,\bar\chi]^{\rm pole}_e$$
$$=\frac{\mu^{-\epsilon}}{(16\pi^2)^2}\int dv_x\left\{\frac{1}{\epsilon^2}\mathrm{tr}(SM\bar M M\bar M)-\left(\frac{1}{\epsilon^2}-\frac{1}{4}\frac{1}{\epsilon}\right)\mathrm{tr}[\nabla_\mu\bar M S\nabla^\mu M]-\frac{1}{\epsilon^2}\mathrm{tr}[S(\bar K+a\bar M)(K+aM)]\right.$$
$$+4\left(\frac{1}{\epsilon^2}+\frac{1}{4}\frac{1}{\epsilon}\right)\lambda_{abc}(\bar M M)^c{}_d\bar\lambda^{dbe}(\bar M M)^a{}_e-i\frac{1}{\epsilon^2}\mathrm{tr}(\bar\Lambda S\not\nabla\Lambda)-2\left(\frac{1}{\epsilon^2}-\frac{3}{4}\frac{1}{\epsilon}\right)a^2\,\mathrm{tr}(S\bar M M)-\frac{13}{30}\frac{1}{\epsilon}a^4\,\mathrm{tr}\,S$$
$$\left.-\frac{1}{2}\left(\frac{2}{\epsilon^2}+\frac{1}{\epsilon}\right)[\lambda_{abc}\lambda_{def}\bar M^{be}\bar M^{cf}(\bar K+a\bar M)^{ad}+\bar\lambda^{abc}\bar\lambda^{def}M_{be}M_{cf}(K+aM)_{ad}]\right\}$$
$$+\frac{i}{16\pi^2}\frac{1}{\epsilon}\int dv_x\left\{-4\lambda_{abc}\bar\lambda^{cde}(\bar M M)^a{}_e H^{Sb}{}_d-\mathrm{tr}(S\Box H^S)+\mathrm{tr}[S\not\nabla^2 H^F]-\frac{i}{2}\mathrm{tr}(S\not\nabla M H^F)-\frac{i}{2}\mathrm{tr}(S\not\nabla\bar M H^F)\right.$$
$$\left.-\lambda_{abc}\lambda_{def}\bar M^{ad}\bar M^{be}H^{cf}-\bar\lambda^{abc}\bar\lambda^{def}M_{ad}M_{be}H^S{}_{cf}\right\}_{\rm diag}\,, \tag{3.37}$$

$$W^{(2)}_{\rm 1PI}[z,z^\dagger,F,F^\dagger,\chi,\bar\chi]^{\rm pole}_f=\frac{1}{2}\frac{\mu^{-\epsilon}}{(16\pi^2)^2}\frac{1}{\epsilon}\int dv_x\{\bar\Lambda'_{ab}\bar\lambda^{bcd}M_{de}\bar\lambda^{eaf}\Lambda_{cf}+\bar\Lambda^{ab}\lambda_{bcd}\bar M^{de}\lambda_{eaf}\Lambda^{cf}\}\,, \tag{3.38}$$

$$W^{(2)}_{\rm 1PI}[z,z^\dagger,F,F^\dagger,\chi,\bar\chi]^{\rm pole}_i$$
$$=\frac{\mu^{-\epsilon}}{(16\pi^2)^2}\int dv_x\left\{2\left(\frac{1}{\epsilon^2}-\frac{1}{4}\frac{1}{\epsilon}\right)\mathrm{tr}(S\bar M M\bar M M)+\frac{2}{\epsilon^2}a^2\,\mathrm{tr}[S\bar M M]+2\left(\frac{1}{\epsilon^2}-\frac{1}{4}\frac{1}{\epsilon}\right)\mathrm{tr}[S(\bar K+a\bar M)(K+aM)]\right.$$
$$\left.+i\left(\frac{1}{\epsilon^2}-\frac{1}{3}\frac{1}{\epsilon}\right)\mathrm{tr}(\bar\Lambda S\not\nabla\Lambda)+\frac{1}{15}\frac{1}{\epsilon}a^4\,\mathrm{tr}\,S\right\}-\frac{1}{2}\frac{i}{16\pi^2}\frac{1}{\epsilon}\int dv_x\{3a^2\,\mathrm{tr}(\bar SH^S)-\mathrm{tr}(\bar S\Box H^S)\}_{\rm diag}\,, \tag{3.39}$$

$$W^{(2)}_{\rm 1PI}[z,z^\dagger,F,F^\dagger,\chi,\bar\chi]^{\rm pole}_k$$
$$=\frac{\mu^{-\epsilon}}{(16\pi^2)^2}\int dv_x\left\{-4\left(\frac{1}{\epsilon^2}-\frac{1}{4}\frac{1}{\epsilon}\right)\mathrm{tr}(S\bar M M\bar M M)+i\left(\frac{1}{\epsilon^2}-\frac{1}{6}\frac{1}{\epsilon}\right)\mathrm{tr}(\bar\Lambda S\not\nabla\Lambda)+2\left(\frac{1}{\epsilon^2}-\frac{1}{2}\frac{1}{\epsilon}\right)\mathrm{tr}(\nabla_\mu\bar M S\nabla^\mu M)\right.$$
$$\left.+4\left(\frac{1}{\epsilon^2}-\frac{1}{2}\frac{1}{\epsilon}\right)a^2\,\mathrm{tr}(S\bar M M)+\frac{11}{30}\frac{1}{\epsilon}a^4\,\mathrm{tr}\,S\right\}-\frac{1}{2}\frac{1}{16\pi^2}\frac{1}{\epsilon}\int dv_x\,\mathrm{tr}[S\not\nabla(i\not\nabla+\mathcal{N})H^F]\,. \tag{3.40}$$

Adding (3.26)–(3.29) and (3.34)–(3.40), we obtain the final result for two-loop divergences:

$$W^{(2)\rm pole}=\frac{\mu^{-\epsilon}}{(16\pi^2)^2}\left(\frac{1}{\epsilon^2}-\frac{1}{2}\frac{1}{\epsilon}\right)\int dv_x\{\mathrm{tr}[\nabla_\mu\bar M S\nabla^\mu M]$$
$$+i\,\mathrm{tr}[\bar\Lambda S\not\nabla\Lambda]+\mathrm{tr}[S(\bar K+a\bar M)(K+aM)]+2a^2\,\mathrm{tr}[S\bar M M]\}\,. \tag{3.41}$$

First we observe that the nonlocal divergences involving H have canceled, demonstrating renormalizability at two-loop order. We also note that the local two-loop divergences have the same form as the one-loop divergences in (2.51) apart from the (possibly fortuitous) absence of a term in a^4. From the discussion following (2.51) we deduce that we may ensure the finiteness of $W^{(2)}$ by taking in $S^{(2)}$

$$Z_A^{(2)} = Z_S^{(2)} = Z_{SA}^{(2)} = Z_F^{(2)} = Z_Q^{(2)} = -\frac{1}{(16\pi^2)^2}\left(\frac{1}{\epsilon^2} - \frac{1}{2}\frac{1}{\epsilon}\right) S^{(2)}, \tag{3.42a}$$

$$w^{(2)} = \frac{-a}{(16\pi^2)^2}\left(\frac{1}{\epsilon^2} - \frac{1}{2}\frac{1}{\epsilon}\right) \times \{\mu^{\epsilon/2} S^a{}_b \bar{\kappa}^{bc} \lambda_{acd} z^d + S^a{}_b \kappa_{ac} \bar{\kappa}^{bc}\}, \tag{3.42b}$$

where

$$S^{(2)a}{}_b = S^c{}_d \bar{\lambda}^{ade} \lambda_{bce}. \tag{3.43}$$

Hence supersymmetry is preserved by the two-loop counterterms. However, precisely as in the one-loop calculation the nonrenormalization theorem fails to hold owing to the necessity for adding a counterterm linear in z to the superpotential w.

IV. CONCLUSION

We have calculated the one- and two-loop divergent counterterms for the Wess–Zumino model defined on a four-dimensional anti-de Sitter space background. We used the version of dimensional regularization proposed by Bellucci and Gonzalez[18] in which the curvature tensor is regarded as residing in four dimensions while all other quantities are analytically extended to $4-\epsilon$ dimensions. This corresponds to regarding the extra dimensions as flat. We demonstrated that this regularization procedure preserves supersymmetry up to two-loop order as far as the counterterms are concerned. We also showed that the superpotential $w(z)$ acquires a divergent contribution linear in the scalar field z at both one and two loops. Hence the nonrenormalization theorem is no longer valid on $(AdS)_4$. This extends the work of Düsedau and Freedman[9] to two-loop order. The divergences of the one-loop one-point functions for z and the auxiliary field F are derived from the linear terms in z and F in (2.51). We immediately confirm the results of Bellucci and Gonzalez for these quantities,[10] and verify the result of Düsedau and Freedman for the one-point function of the scalar field after eliminating F by means of its equation of motion.

The method we used has the advantages of obtaining results for divergences relatively speedily and systematically, but, on the other hand, since it is not explicitly supersymmetric there is no guarantee that it will be useful for calculating the finite contributions. An explicitly supersymmetric procedure for performing two-loop calculations while retaining the simplicity and elegance of the heat kernel method has recently been suggested by Abdalla and Abdalla.[28] They expand the Green's function in terms of the heat kernel coefficients in a similar fashion to (3.5), but use a nonzero lower limit of integration in (3.4) as a cutoff, instead of analytically continuing in d. It seems likely that a calculation using this method would be formally similar to ours and yield corresponding results for the two-loop divergences. It would be interesting to determine whether the expectation value of F is zero at two loops using an explicitly supersymmetric regulator as seems indicated by the similarity of the one- and two-loop counterterms.

Note added in proof: Recently our attention was drawn[30] to the fact that the Green's functions we use do not explicitly satisfy the appropriate boundary conditions for $(AdS)_4$ (see Ref. 31). We believe that the short-distance behavior of the Green's functions leading to the divergences we have computed is unaffected by the boundary conditions; however, there remains the possibility of additional divergences arising from antipodally separated points, and this is currently under investigation.

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APPENDIX: SCHWINGER–DE WITT KERNEL IDENTITIES

In this Appendix we shall list some useful identities for the kernel coefficients $a_n^\Delta(x,x')$, which appear in the asymptotic expansion (2.38) of the Schwinger–De Witt kernel for an operator of the form (2.36).

By substituting the expansion (2.38) into the defining equation (2.37) for the Schwinger–De Witt kernel, we find the recurrence relations

$$\sigma_{;\mu} D^\mu a_0^\Delta(x,x') = 0, \tag{A1a}$$

$$n a_n^\Delta(x,x') + \sigma^\mu D_\mu a_n^\Delta(x,x') = -\Delta_{\rm VM}^{-1/2}\Delta\left[\Delta_{\rm VM}^{1/2} a_{n-1}^\Delta(x,x')\right]. \tag{A1b}$$

By iterative solution of this equation we may readily obtain expressions for the coincidence limits of the coefficients a_n^Δ and their covariant derivatives (after using results for the coincidence limits of derivatives of $\Delta_{\rm VM}$ and σ given elsewhere.[14,24,29] The most useful results for our purposes are as follows:

$$(a_0{}^\Delta)_{\rm diag} = \mathbf{1}^\Delta, \tag{A2a}$$

$$(a_1{}^\Delta)_{\rm diag} = -2a^2\mathbf{1}^\Delta - Y^\Delta, \tag{A2b}$$

$$(D_\beta D_\alpha a_1{}^\Delta)_{\rm diag} = -\tfrac{1}{12}(G^\Delta_{\alpha\mu} G^\Delta{}_\beta{}^\mu + G^\Delta_{\beta\mu} G^\Delta{}_\alpha{}^\mu) + \tfrac{1}{3} G^\Delta_{\alpha\beta}(2a^2\mathbf{1}^\Delta + Y^\Delta) + \tfrac{1}{6}(2a^2\mathbf{1}^\Delta + Y^\Delta) G^\Delta_{\alpha\beta} + \tfrac{1}{30} a^4 g_{\alpha\beta}\mathbf{1}^\Delta - \tfrac{1}{3}\mathscr{D}_\beta \mathscr{D}_\alpha Y^\Delta, \tag{A2c}$$

$$(a_2{}^\Delta)_{\rm diag} = \tfrac{1}{12} G^\Delta_{\alpha\beta} G^{\Delta\alpha\beta} + \tfrac{1}{2}(2a^2\mathbf{1}^\Delta + Y^\Delta)^2 - \tfrac{1}{15} a^4 \mathbf{1}^\Delta + \tfrac{1}{6}\mathscr{D}^2 Y^\Delta, \tag{A2d}$$

where $\mathscr{D}_\alpha$ and $G^\Delta_{\alpha\beta}$ are defined in (2.42). Two useful results for the coincidence limits of the Green's function G_Δ in (3.5), and its covariant derivatives, are as follows:

$$G_{\Delta\rm diag} = -i\frac{2}{\epsilon}\frac{\mu^{-\epsilon}}{16\pi^2} a_1{}^\Delta{}_{\rm diag} + H^\Delta{}_{\rm diag}, \tag{A3a}$$

$$(D^2 G_\Delta)_{\rm diag} = -i\frac{2}{\epsilon}\frac{\mu^{-\epsilon}}{16\pi^2}\left\{D^2 a_1^\Delta + \frac{1}{2}da_2^\Delta - \frac{1}{6}Ra_1^\Delta\right\}_{\rm diag} + (D^2 H^\Delta)_{\rm diag}\,. \tag{A3b}$$

Finally a word is in order about the transition from Euclidean to Lorentzian signature. The functional integral e^{iW} defining a field theory on a space-time with signature $(+,-,-,-)$ may be obtained from the functional integral e^{-W} defining the theory on a space-time with Euclidean signature by replacing x_4 by ix_0. As a consequence the fundamental relation,[16] from which we obtain the residues of the poles in ϵ arising from products of functions of the type G_0 or R_n in (3.6), takes the form

$$\frac{1}{(-2\sigma)^{(1/2)(d-\delta)}} \sim \frac{\mu^{-\epsilon}}{\delta}\frac{2\pi^{(1/2)d}}{\Gamma(\frac{1}{2}d)}\delta^d\,, \tag{A4}$$

for $\delta = O(\epsilon)$.

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Generalized conditions for the decoupling theorem of quantum field theory in Minkowski space with particles of vanishingly small masses

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The proof of the decoupling theorem of quantum field theory given earlier [E. B. Manoukian, J. Math. Phys. **26**, 1065 (1985)] in *Minkowski* space, in the distributional sense, for theories involving particles with vanishingly small masses as well is extended under more general conditions, thus being applicable to a larger class of graphs. All subtractions of renormalization are carried out at the origin of momentum space with the degree of divergence of a subtraction coinciding with the dimensionality of the corresponding subdiagram.

I. INTRODUCTION

In an earlier paper,[1] referred to as (I), a proof of the decoupling theorem of quantum field theory was given in Minkowski space, in the distributional sense, for theories with particles of vanishingly small masses under sufficiency conditions. These sufficiency conditions are stated in Theorem 1 (Sec. II). In the present paper, the theorem is proved (Theorem 2) under more *general* conditions thus extending the validity of the decoupling theorem to a larger class of graphs involving particles of vanishingly small masses. The theorem establishes the vanishing of the renormalized Feynman amplitudes in Minkowski space, in the distributional sense, when any subset of the masses become *large* and some of the remaining masses are scaled down to zero. The study is very general in that we allow these masses to approach their asymptotic values at different rates. Extensive use is made of a key estimate established in (I) that bounds the amplitudes in *Minkowski* space by similar amplitudes in Euclidean space in absolute values. The theorem established in Minkowski space is also applicable in Euclidean space with nonexceptional external momenta. All the subtractions of renormalization are carried out in momentum space about the origin with the degree of divergence $d(g)$ associated with a subtraction coinciding with the dimensionality of the corresponding subdiagram g.

II. PROOF OF THE THEOREM

Suppose G is a proper and connected graph. Let $\mu=\{\mu^1,...,\mu^s,\mu^{s+1},...,\mu^{s+k},\mu^{s+k+1},...,\mu^\rho\}$ denote the set of masses in G, where $\mu^i>0$, $i=1,2,...,\rho$. We are interested in studying the limits

$$\lim_{\substack{\xi_1,...,\xi_k\to\infty\\ \lambda_1,...,\lambda_s\to 0}}\left(\lim_{\epsilon\to+0} T^{(\epsilon)}_{\xi_1,...,\xi_k;\lambda_1,...,\lambda_s}(f)\right), \tag{1}$$

where

$$T^{(\epsilon)}_{\xi_1,...,\xi_k;\lambda_1,...,\lambda_s}(f) = \int_{\mathbb{R}^{4m}} dP f(P)\int_{\mathbb{R}^{4n}} dK \times R_\epsilon(P,K,\lambda_1\mu^1,...,\lambda_1\cdots\lambda_s\mu^s, \xi_1\cdots\xi_k\mu^{s+1},...,\xi_k\mu^{s+k},\mu^{s+k+1},...,\mu^\rho), \tag{2}$$

where R_ϵ is the renormalized (subtracted out) Feynman integrand associated with G, and $P=\{p_1^0,...,p_m^3\}$, $K=\{k_1^0,...,k_n^3\}$ denote, respectively, the set of external and internal (independent) momenta. Here $f(P)\in\mathcal{S}(\mathbb{R}^{4m})$ is a Schwartz function. For $\epsilon>0$, $\lambda_1\neq 0,...,\lambda_s\neq 0$, $1\leqslant\xi_1<\infty,...,1\leqslant\xi_k<\infty$, the integral in (2) is absolutely convergent. Here $R_\epsilon(P,K,\mu)$ has the familiar form

$$R_\epsilon(P,K,\mu)=A(P,K,\mu)\prod_{l=1}^{L} D_l^{-1},\quad \epsilon>0, \tag{3}$$

$$D_l=Q_l^2+\mu_l^2-i\epsilon(\mathbf{Q}_l^2+\mu_l^2),\quad \mu_l>0, \tag{4}$$

$$Q_l=\sum_{i=1}^{m} a_{li}p_i+\sum_{j=1}^{n} b_{lj}k_j\equiv p^l+k^l, \tag{5}$$

where $\mu_l\in\mu$, and A is a polynomial in its argument and may, in general, be a polynomial in $(\mu^{s+1})^{-1},...,(\mu^\rho)^{-1}$ as well. A propagator carrying a momentum Q_l will be written in the form

$$D^+(Q_l,\mu_l)=(\mu_l)^{-\delta_l}\frac{\tilde{P}(Q_l,\mu_l)}{[Q_l^2+\mu_l^2-i\epsilon(\mathbf{Q}_l^2+\mu_l^2)]},\quad \mu_l>0, \tag{6}$$

where, for $\mu_l\in[\mu^1,...,\mu^s]$, $\delta_l\equiv 0$, and for $\mu_l\in[\mu^{s+1},...,\mu^\rho]$, δ_l is some non-negative integer. The latter is well known for massive higher spin fields, and where $\tilde{P}(Q_l,\mu_l)$ is a polynomial in μ_l. For $\mu_l\in[\mu^1,...,\mu^s]$, $D^+(Q_l,0)$ denotes the zero-mass propagator. We assume throughout that

$$\operatorname*{degr}_{\mu_l} D^+(Q_l,\mu_l)\leqslant -1, \tag{7}$$

$$\operatorname*{degr}_{Q_l,\mu_l} D^+(Q_l,\mu_l)<\operatorname*{degr}_{Q_l} D^+(Q_l,\mu_l). \tag{8}$$

The $\epsilon\to+0$ limit in (1) establishes[2] the existence of the renormalized Feynman amplitudes in Minkowski space in the distributional sense.

In (I) the following theorem is established.

Theorem 1: Suppose (a) there are no proper, connected, and divergent $[d(g)\geqslant 0]$ subdiagrams $g\subset G$ such that all the masses in g are from the set $\{\mu^1,...,\mu^s\}$; and (b) any subdiagram $G'\subseteq G$, where G/G' depends solely on the masses in the set $\{\mu^1,...,\mu^s\}$, is such that $d(G')<d(G)$. Then

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$$\lim_{\substack{\xi_1,\ldots,\xi_k\to\infty \\ \lambda_1,\ldots,\lambda_s\to 0}} \left(\lim_{\epsilon\to+0} T^{(\epsilon)}_{\xi_1,\ldots,\xi_k;\lambda_1,\ldots,\lambda_s}(f) \right) = 0, \tag{9}$$

for all $f(P)\in\mathcal{S}(\mathbb{R}^{4m})$, and where the limits $\xi_1,\ldots,\xi_k\to\infty$, $\lambda_1,\ldots,\lambda_s\to 0$ are taken independently.

Here we recall that G is a proper and connected graph. The symbol $\subset$ may include equality, and the symbol $\not\subset$ excludes equality. Here G/G' represents the graph G with G' shrunk in it to a point.

The application of Theorem 1 is simple as it requires no computations whatsoever and all that it requires is a mere examination of the structure of the graph G. For example, let G denote the electron self-energy graph in quantum electrodynamics, in any order, without photon self-energy insertions, with m denoting the electron mass and μ denoting a photon mass. We note the following: (a) there are no proper (and connected and divergent) subdiagrams $g\subset G$ (including G itself) consisting solely of photon lines; and (b) for any subdiagram $G'\not\subset G$, such that G/G' consists solely of photon lines we necessarily have $d(G')<d(G)$ $(=1)$. Hence the conditions in Theorem 1 are true and if we scale m by ξ and μ by λ, and take the limits $\xi\to\infty$, $\lambda\to 0$, the statement in (9) follows for the graph G. We note, however, that once we insert a photon self-energy graph in G, then we may create a subdiagram G' in G such that G/G' consists solely of photon lines and $d(G')=d(G)$. Hence Theorem 1 is not directly applicable, but the statement in (9) still holds true as seen from the following theorem.

In order to state Theorem 2, we denote by G_0 any connected and amputated graph with only two external lines to G_0 such that the mass (or masses) in the two external lines to G_0 are from the set $\{\mu^1,\ldots,\mu^s\}$. Any such subdiagram will be called a G_0 graph. By attaching the two external lines, with corresponding propagators $D_0^+(Q)$, to a G_0 graph, we generate an unamputated graph which we denote by G_0' and refer to it as a G_0' graph. We assume that

$$d(G_0') = d(G_0) + 2\deg_Q D_0^+(Q) \leqslant -1. \tag{10}$$

We note that for $G_0\not\subset G$ (or $G_0'\not\subset G$) the external two lines to G_0 (or of G_0') are necessarily internal lines in G, since G is proper.

Theorem 2: Suppose the following hold.

(a) There are no proper, connected, and divergent $[d(g)\geqslant 0]$ subdiagrams $g\subset G$ such that all the masses in g are from the set $\{\mu',\ldots,\mu^s\}$.

(b) Let G' be *any* subdiagram $G'\not\subset G$, where G/G' depends *solely* on masses from the set $\{\mu^1,\ldots,\mu^s\}$. Suppose that for all such subdiagrams G', we have the following.

(i) If none of the connected components of G' are G_0 graphs (or G_0' graphs) then $d(G')<d(G)$.

(ii) If one or more the connected components of G' are G_0 graphs (or G_0' graphs), let G_1' denote the union of the connected components of G' involving *no* G_0'-components, then

$$0\leqslant d(G) \text{ if } G_1'=\varnothing;\ d(G_1')<d(G) \text{ if } G_1'\neq\varnothing.$$

If the above conditions (a) and (b) are true then (9) follows.

The above theorem is easy to apply as again it involves no computations, and it only requires a mere examination of the structure of the proper and connected graph G in question. Examples will be given later.

To prove Theorem 2, we need the following. Consider the elements in P,K,μ as the components[1] of a vector $\mathbf{P}'$ in $\mathbb{R}^{4m+4n+\rho}$. Suppose $\mathbf{P}'$ is of the form

$$\mathbf{P}' = \sum_{i=1}^{t} \mathbf{L}_i'\eta_i\eta_{i+1}\cdots\eta_t + \mathbf{C}', \qquad t\in[1,\ldots,(4m+4n+\rho)], \tag{11}$$

where $\mathbf{L}_1',\ldots,\mathbf{L}_t'$ are t independent vectors in $\mathbb{R}^{4m+4n+\rho}$, $\mathbf{C}'$ is a vector confined to a finite region in $\mathbb{R}^{4m+4n+\rho}$, and $\eta_1>1,\ldots,\eta_t>1$ are some parameters. In reference to the graph G, we write $Q_l=p^l+k^l$ [see Eq. (5)], for the momentum Q_l carried by a line l in G. Suppose that for some l, k^l depends on the parameter η_r, for r fixed in $[1,\ldots,t]$. Then we may write R_ϵ in (2) in a familiar form[1,3]:

$$R_\epsilon = \sum_{\mathcal{N}} \prod_{g\in\mathcal{N}} (\delta_g^{\mathcal{N}} - T_g) I_G, \tag{12}$$

where the sum is over all $\mathcal{N}$ sets of proper, connected subdiagrams such that we have the following.

(i) $G\in\mathcal{N}$.

(ii) If $g_1,g_2\in\mathcal{N}$, then either $g_1\cap g_2=\varnothing g_2$ or $g_1\not\subset g_2$ or $g_2\not\subset g_1$.

(iii) Let $g\in\mathcal{N}$. If $g_1,\ldots,g_m$ denote the maximal elements in $\mathcal{N}$ contained in g: $g_i\not\subset g$, $i=1,\ldots,m$, then define $\bar g = g/(g_1\cup g_2\cup\cdots\cup g_m)$ by shrinking $g_1,\ldots,g_m$ in g to points. Then all the $(k^l)^g$ (which are linear combinations of the integration variables in K) of $\bar g$ are either all dependent on η_r or are all independent of η_r.

Also (a) $\delta_G^{\mathcal{N}}=1$; (b) if $g\not\subset G$ in $\mathcal{N}$, and all the $(k^l)^g$ of $\bar g$ are independent of η_r, then $\delta_g^{\mathcal{N}}=0$; (c) if g is one of the maximal elements in $\mathcal{N}$ contained in a subdiagram $g'\in\mathcal{N}$, such that all $(k^l)^{g'}$ of $\bar g'$ are independent of η_r, and all the $(k^l)^g$ of $\bar g$ are dependent on η_r, then $\delta_g^{\mathcal{N}}=1$; and (d) if $g\in\mathcal{N}$ $(g\not\subset G)$ is one of the maximal elements contained in $g'\in\mathcal{N}$ such that all the $(k^l)^{g'}$ of $\bar g'$ are dependent on η_r, then $\delta_g^{\mathcal{N}}=0$. If $d(g)<0$, then $T_g\equiv 0$, for the Taylor operation, by definition.

We write

$$\mathcal{N} = \mathcal{H}_1\cup\mathcal{H}_2, \tag{13}$$

where $g\in\mathcal{H}_1$ if all the $(k^l)^g$ of $\bar g$ are dependent on η_r, and $g\in\mathcal{H}_2$ if all the $(k^l)^g$ of $\bar g$ are independent of η_r. We also write

$$\mathcal{H}_1 = \mathcal{F}_1\cup\mathcal{F}_2, \tag{14}$$

where for $g\in\mathcal{H}_1$, with $g\not\subset G$, $g\in\mathcal{F}_1$ if $\delta_g^{\mathcal{N}}=0$, and $g\in\mathcal{F}_2$ if $\delta_g^{\mathcal{N}}=1$. Equation (12) may be then also rewritten as[3]

$$R_\epsilon = \sum_{\mathcal{N}} F_G(\mathcal{N}), \tag{15}$$

where we have recursively

$$F_g(\mathcal{N}) = (\delta_g^{\mathcal{N}} - T_g) I_{\bar g} \prod_i F_{g_i}(\mathcal{N}), \tag{16}$$

and $\{g_i\}_i$ denotes the set of maximal elements in $\mathcal{N}$ contained in g: $g_i\not\subset g$. The maximal elements in $\mathcal{N}$ contained in G will be denoted by $G_1,\ldots,G_m$: $G_i\not\subset G$.

To prove Theorem 2, consider a scale parameter $1/\lambda_i$, and suppose that the latter is scaled by a parameter η_r [see Eq. (11)]. Three possibilities may arise: either all ([A]) or some ([B]) or none ([C]) of the k^l in G depend on η_r. We treat all cases. We use the notation

$$\sigma(g)=4\sum_{\substack{g'\in\mathscr{H}_1\\ g'\subset g}}L(\bar{g}'), \tag{17}$$

where $L(g)$ denotes the number of independent loops in g.

[A] Suppose $G\in\mathscr{F}_2$, then, according to (I),

$$\operatorname*{degr}_{\eta_r} F_G(\mathscr{N})\leqslant d(G)-\sigma(G), \tag{18}$$

where $\sigma(G)=4L(G)=4n$.

[B] Suppose $G\in\mathscr{H}_2$, then, for $d(G)\geqslant 0$ [1],

$$\operatorname*{degr}_{\eta_r}(-T_G)I_{\bar{G}}\prod_{i=1}^{m}F_{G_i}(\mathscr{N})<d(G)-\sigma(G), \tag{19}$$

and no equality in (19) may arise. Let G' be the subdiagram G' in G such all the lines in $G'/(G_1\cup\cdots\cup G_m)$ depend on η_r and G/G' is independent of η_r. Then from (I)

$$\begin{aligned}&\operatorname*{degr}_{\eta_r} I_{\bar{G}}\prod_{i=1}^{m}F_{G_i}(\mathscr{N})\\ &\quad<d(G')-4L(\bar{G}')-\sum_{i=1}^{m}\sigma(G_i)\\ &\quad\begin{cases}=d(G')-\sigma(G), & \text{if } L(\bar{G}')=0,\\ <d(G')-\sigma(G), & \text{if } L(\bar{G}')\neq 0.\end{cases}\end{aligned} \tag{20}$$

If $G'\equiv G$, then $L(\bar{G}')\neq 0$, and we have from (20)

$$\operatorname*{degr}_{\eta_r} I_{\bar{G}}\sum_{i=1}^{m}F_{G_i}(\mathscr{N})<d(G)-\sigma(G), \tag{21}$$

and no equality may hold in (21). Now consider the case $G'\not\subseteq G$

(i) If none of the connected components of G' are G_0' graphs (or G_0 graphs), then from condition (b) (i) in Theorem 2, $d(G')<d(G)$, and from (20), the inequality in (21) again holds true and no equality may arise in it.

(ii) If G' has one or more G_0' graphs as one or more of its connected components, then, without loss of generality, suppose that G' has only one G_0' component, and write $G'=G_0'\cup G_1'$, where none of the connected components of G_1' are G_0' graphs (or G_0 graphs).

Let $G_1^0,\ldots,G_t^0$ be those elements in the set $\{G_1,\ldots,G_m\}$ falling in G_0': $G_i^0\not\subseteq G_0'$, $i=1,\ldots,t$. Suppose all the external momenta of $G_1^0,\ldots,G_t^0$ are independent of η_r. Then the subtraction formalism guarantees[3] that

$$\begin{aligned}&\operatorname*{degr}_{\eta_r} F_{G_i^0}(\mathscr{N})\leqslant\min[d(G_i^0),-1]-\sigma(G_i^0),\\ &\quad i=1,\ldots,t.\end{aligned} \tag{22}$$

Also all the η_r dependence in $G_0'/(G_1^0\cup\cdots\cup G_t^0)$ will then come from the masses in the latter subdiagram, that is from (22) and (7):

$$\operatorname*{degr}_{\eta_r} I_{\bar{G}_0'}\prod_{i=1}^{t}F_{G_i^0}(\mathscr{N})\leqslant -1-\sum_{i=1}^{t}\sigma(G_i^0). \tag{23}$$

On the other hand if some of the external momenta of one or more of the $G_1^0,\ldots,G_t^0$ depend on η_r, then by momentum conservation, the external momenta of G_0' depend on η_r (that is we will be dealing with a G_0' graph rather than a G_0 graph). Hence from (20) and (10), the inequality in (23) again holds true. Therefore, *if* $G_1'=\emptyset$, $\{G_1^0,\ldots,G_t^0\}\equiv\{G_1,\ldots,G_m\}$, *and* $d(G)\geqslant 0$ [see condition (b) (ii) in Theorem 2] we have from (23) that

$$\operatorname*{degr}_{\eta_r} I_{\bar{G}}\prod_{i=1}^{m}F_{G_i}(\mathscr{N})<d(G)-\sigma(G). \tag{24}$$

If $G_1'\neq\emptyset$, then by definition G_1' contains no G_0' components (or G_0 components) and hence from part (b) (i) in Theorem 2, $d(G_1')<d(G)$, that is

$$\operatorname*{degr}_{\eta_r} I_{\bar{G}_1'}\prod_{i=1}^{r}F_{G_i^1}(\mathscr{N})<d(G)-\sum_{i=1}^{r}\sigma(G_i^1), \tag{25}$$

where $G_1^1,\ldots,G_r^1$ are the elements in $\{G_1,\ldots,G_m\}$ falling in G_1'. From (23) and (25), we then conclude that the inequality in (24) again holds true and no equality may arise in it.

Hence for case [B], with $G\in\mathscr{H}_2$,

$$\operatorname*{degr}_{\eta_r} F_g(\mathscr{N})<d(G)-\sigma(G), \tag{26}$$

and no equality may arise in (26).

[C] Suppose that all the k^l in G are independent of η_r. Then (for $d(G)\geqslant 0$)

$$\operatorname*{degr}_{\eta_r}(-T_G)\cdots I_G<d(G), \tag{27}$$

where we have used (7) and (8). Also for $G''\not\subseteq G$, with G'' proper and divergent,

$$\operatorname*{degr}_{\eta_r} I_{\bar{G}}(-T_{G''})\cdots I_{G''}\leqslant d(G')-4L(G'/G''), \tag{28}$$

where G/G' (if not empty) is independent of η_r. If $G'\equiv G$, then $L(G/G'')\neq 0$, and (27) and (28) imply that

$$\operatorname*{degr}_{\eta_r} R<d(G). \tag{29}$$

Suppose $G'\not\subseteq G$. If G' has *no* G_0' components as one or more of its connected components, then $d(G')<d(G)$, by condition (b) (i) in Theorem 2, and (29) holds true with no equality arising in it, as seen from (27) and (28). Otherwise suppose that $G'=G_0'\cup G_1'$, where, without loss of generality, we consider the case when G' has only one G_0' component. Then, according to condition (b) in Theorem 2,

$$\begin{aligned}&d(G')=d(G_0')+d(G_1')\leqslant -1+d(G_1')\\ &\qquad\begin{cases}<d(G), & \text{if } G_1'\neq\emptyset,\\ <d(G), & \text{if } d(G)\geqslant 0,\quad G_1'=\emptyset,\end{cases}\end{aligned} \tag{30}$$

where we have used the condition that if the external momenta of G_0' are independent of η_r, then its masses must depend on η_r and hence (7); on the other hand if the external momenta of G_0' depend on η_r, then we may use (10). Hence in case [C] no equality may arise in (29).

According to (I) and the derived estimates in [A], [B], and [C] [see, in particular, Eqs. (31)–(39), and Eq. (10) in (I)], we may bound the amplitudes in Minkowski space as

$$|\hat{T}_{\xi_1,\ldots,\xi_k;\lambda_1,\ldots,\lambda_s}(f)|$$

$$\leqslant C\frac{1}{\xi_1\cdots\xi_k}\mathscr{P}(\ln\xi_1,\ldots,\ln\xi_k)$$

$$\times(\lambda_1\cdots\lambda_s)^{d(G)+4m-2N}\prod_{i=1}^{s}\left(\frac{1}{\lambda_i}\right)^{d(G)+4m-2N} \quad (31)$$

or

$$|\hat{T}_{\xi_1,\ldots,\xi_k;\lambda_1,\ldots,\lambda_s}(f)|$$

$$\leqslant C\frac{1}{\xi_1\cdots\xi_k}\mathscr{P}(\ln\xi_1,\ldots,\ln\xi_k)\to 0, \quad (32)$$

for $\xi_1,\ldots,\xi_k\to\infty$, $\lambda_1,\ldots,\lambda_s\to 0$, where $\mathscr{P}(\ln\xi_1,\ldots,\ln\xi_k)$ is some polynomial in $\ln\xi_1,\ldots,\ln\xi_k$, and no logarithmic growth occurs in (31) and (32) in the parameters $1/\lambda_i$, $i=1,\ldots,s$; N is some large positive integer, and[1,2]

$$\lim_{\epsilon\to+0} T^{(\epsilon)}_{\xi_1,\ldots,\xi_k;\lambda_1,\ldots,\lambda_s}(f)=\hat{T}_{\xi_1,\ldots,\xi_k;\lambda_1,\ldots,\lambda_s}(f). \quad (33)$$

This completes the proof of Theorem 2.

As an example, consider the electron self-energy graph G in quantum electrodynamics, in any order, *with* photon self-energy insertions. We note (a) G contains no proper (connected and divergent) subdiagrams consisting solely of a photon line, and (b) let G_0 be a photon self-energy graph insertion in G. Hence (10) is true, and any subdiagram $G_1'\subsetneq G$, not having a photon self-energy graph as one of its connected parts, such that $G/(G_0\cup G_1')$ consists solely of photon lines is such that $d(G_1')<d(G)(=1)$. Accordingly, the conditions in (a) and (b) in Theorem 2 are true and hence (9) holds also true for the graph G when the electron mass m is scaled by a parameter ξ, and a photon mass μ is scaled by a parameter λ, and the limits $\xi\to\infty$, $\lambda\to 0$ are taken. As another example, consider the photon self-energy graph, to any order, with photon self-energy insertions. It is readily checked that the conditions (a) and (b) in Theorem 2 are satisfied and hence (9) also holds true.

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Intrinsic nonlinear spinor wave equations associated with nonlinear spinor representations

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New covariant nonlinear spinor wave equations associated with nonlinear spinor representations of pseudo-orthogonal groups are derived. The wave equations obtained possess specific nonlinearities, which, in the intrinsic spinor coordinates, have the form of bilinear nonlinearities. Due to the existence of a large number of natural constraints, typical for nonlinear spinor representations, the number of independent spinor components in the present theory is considerably reduced.

I. INTRODUCTION

The most interesting supersymmetric[1] and superstring[2] field theories are currently constructed in a space-time of 10 or 11 dimensions. However, many attractive features of higher-dimensional space-time field theories are diminished by the fact that in these cases the number of independent covariant spinor components is very high.

We demonstrated in a previous work[3] that in higher-dimensional space-times there exists—besides the well-known linear irreducible spinor representation—a specific nonlinear spinor representation for which the number of independent spinor components are restricted in a natural manner by quadratic covariant contraints. For instance, for the $SO(\nu,\nu)$ pseudo-orthogonal groups the number of spinor components in the linear representation is $2^{\nu-1}$, whereas the number of independent spinor components for the nonlinear representation is $1+\binom{\nu}{2}$: this gives, e.g., for $\nu=10$, 512 spinor components for the linear representation, versus 46 for the nonlinear one. Hence the nonlinear spinors may form the natural minimal "building blocks" for field theories in higher-dimensional space-times.[4]

In this work we consider the field theory associated with the nonlinear spinor representations of $SO(\nu,\nu)$ and $SO(\nu+1,\nu)$. We show that the Dirac-like, covariant wave equation

$$\Gamma^a \partial_a \psi(x)=0, \quad x\in\mathbb{R}^{\nu,\nu}, \quad \text{or} \quad \mathbb{R}^{\nu+1,\nu}, \tag{1.1}$$

where Γ^a are the generators of the corresponding Clifford algebra, reduces to a unique system of nonlinear field equations for independent spinor components with quadratic nonlinearities. Thus even the simplest theory with one spinor field, transforming according to a nonlinear spinor representation, represents a highly nontrivial specific nonlinear field theory.

One can consider the resulting nonlinear field theory as a σ-type model spinor field theory.[5] In fact the spinor ψ of, e.g., $SO(\nu,\nu)$ satisfies a set of $2^{\nu-1}-1-\binom{\nu}{2}$ quadratic constraints

$$\tilde{\psi}\Gamma_{a_1\cdots a_k}\psi=0, \quad \text{for } k=0,1,\ldots,\nu-1, \tag{1.2}$$

where $\Gamma_{a_1\cdots a_k}$ are polyvectors generated by Γ_a. Then Eq. (1.1) together with (1.2) represents in fact a spinor-type nonlinear σ-model.[5]

In this work we concentrate on the derivation of nonlinear spinor wave equations associated with (1.1) for the $SO(\nu,\nu)$ and $SO(\nu+1,\nu)$ groups. In Sec. II, we give a detailed analysis of the properties of these equations for the $SO(\nu,\nu)$ and in Sec. III for the $SO(\nu+1,\nu)$ groups. In Sec. IV, we call attention to the interesting fact that the nonlinear spinor representation considered in this work represents one out of the whole set of nonlinear spinor representations associated with a given linear spinor representation of the $SO(p,q)$ group. We show that, choosing properly the standard pure spinors $\overset{k}{\psi}$ with a stability group $\overset{k}{H}$, we obtain a whole sequence of nonlinear spinor representations $\overset{k}{T}$, whose carrier spaces $\overset{k}{N}{}^m$ will be isomorphic with the homogeneous spaces

$$\overset{k}{C}=SO(p,q)/\overset{k}{H}.$$

In this language the present nonlinear (pure spinor) representation of the $SO(\nu,\nu)$ and $SO(\nu+1,\nu)$ group corresponds to the stability subgroup $\overset{1}{H}$ of

$$\overset{1}{\psi}=\begin{Vmatrix}1\\0\\\vdots\\0\end{Vmatrix}. \tag{1.3}$$

This nonlinear spinor represenation has the smallest dimension, since the stability group $\overset{1}{H}$ is the largest possible. All remaining nonlinear spinor representations will have dimension d_k with $1+\binom{\nu}{2}<d_k<2^{\nu}$. One can extend the present

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theory to these nonlinear spinor representations and one gets the corresponding nonlinear wave equations.

In Sec. V we summarize the obtained results and present some interesting research problems connected with coupling of nonlinear spinors with other fields and with a second quantization of spinor field theories associated with nonlinear spinor representations.

II. COVARIANT WAVE EQUATIONS FOR SO(ν,ν) PURE SPINORS

The pseudo-orthogonal group $SO(\nu,\nu)$ is most naturally realized in the $\mathbb{R}^{\nu,\nu}$ pseudo-Euclidean space with a coordinate system such that the metric tensor is given by

$$g = \{g_{ab}\} = \left|\left| \begin{matrix} \mathbf{1}_\nu & 0 \\ 0 & -\mathbf{1}_\nu \end{matrix} \right|\right|,$$

$$a,b = 1,...,2\nu.$$

However, as Cartan demonstrated,[6] the analysis of spinor representations is most effectively carried out in an isotropic coordinate system obtained from the previous one by the transformation

$$r = \frac{1}{2}\left|\left| \begin{matrix} \mathbf{1}_\nu & \mathbf{1}_\nu \\ \mathbf{1}_\nu & -\mathbf{1}_\nu \end{matrix} \right|\right|.$$

The coordinates corresponding to $x = (x_\mu) \in \mathbb{R}^{\nu,\nu}$ are y^l and $y^{l'}$, $l,l' = 1,...,\nu$, and the metric tensor has the form

$$\tilde{g} = \{\tilde{g}_{rs}\} = \frac{1}{2}\left|\left| \begin{matrix} 0 & \mathbf{1}_\nu \\ \mathbf{1}_\nu & 0 \end{matrix} \right|\right|,$$

$$r,s = 1,...,\nu,1',...,\nu'. \tag{2.1}$$

If Γ_a, $a = 1,...,2\nu$ are basis elements of the Clifford algebra

$$\{\Gamma_a,\Gamma_b\} = 2g_{ab}\mathbf{1}_{2\nu}, \quad a,b = 1,...,2\nu,$$

associated with the $\mathbb{R}^{\nu,\nu}$ space, then the new basis for the Clifford algebra is given by

$$H_l = \tfrac{1}{2}(\Gamma_{2l-1} + \Gamma_{2l}), \quad H_{l'} = \tfrac{1}{2}(\Gamma_{2l-1} - \Gamma_{2l}),$$

$$l = 1,...,\nu,$$

satisfying the relation

$$\{H_r,H_s\} = 2\tilde{g}_{rs}\mathbf{1}_{2\nu}, \quad r,s = 1,...,\nu,1',...,\nu'. \tag{2.2}$$

The semispinor ψ from the carrier space L^{m_+} of the irreducible linear representation of $SO(\nu,\nu)$ of dimension $2^{\nu-1}$, corresponding to the highest weight $m_+ = (\frac{1}{2},...,\frac{1}{2})$, can be represented as a column, where all components with an odd number of indices are zero, i.e.,

$$\psi = \left\| \begin{matrix} \psi_0 \\ 0 \\ \vdots \\ \psi_{12} \\ \vdots \\ \psi_{\nu-1\nu} \\ 0 \\ \vdots \\ 0 \\ \psi_{i_1 \cdots i_{2[\nu/2]}} \end{matrix} \right\|. \tag{2.3}$$

As shown by Cartan,[6] $\psi_{i_1 \cdots i_{2p}}$, $1 \leqslant p \leqslant [\nu/2]$, are totally antisymmetric in $i_1,...,i_{2p}$. From Ref. 7, we have that $\psi_{i_1 \cdots i_{2p}}$ for $2 \leqslant p \leqslant [\nu/2]$ are given in terms of ψ_0 and $\psi_{i_1 i_2}$ by the formula

$$\psi_{i_1 \cdots i_{2p}} = (2p-1)!!\psi_0^{1-p}\psi_{[i_1 i_2} \cdots \psi_{i_{2p-1} i_{2p}]}, \tag{2.4}$$

where we have introduced the notation for totally antisymmetric tensors

$$T_{[i_1 \cdots i_r]} := \frac{1}{r!}\sum_{\pi(i_1,...,i_r)} (-1)^\pi T_{i_{\pi_1} \cdots i_{\pi_r}}, \tag{2.5}$$

with the summation extended over all permutations of the indices $i_1,...,i_r$ and $(-1)^\pi$ denoting the signature of the given permutation.

We now consider the covariant Dirac-like equation for the pure spinor $\psi(x)$ in the $\mathbb{R}^{\nu,\nu}$ space

$$\Gamma^a \frac{\partial}{\partial x^a}\psi(x) = 0. \tag{2.6a}$$

This equation looks like a linear equation in the components $\psi_{i_1 \cdots i_{2p}}$, $p = 0,1,...,[\nu/2]$; however, due to the constraints (2.4), it is equivalent to a specific set of nonlinear equations with quadratic nonlinearities. To show this, we pass to Cartan coordinates in which (2.5) has the form

$$\sum_{l=1}^{\nu}\left(H_l \frac{\partial}{\partial y_l} + H_{l'}\frac{\partial}{\partial y_{l'}}\right)\psi(y) = 0. \tag{2.6b}$$

The derivatives $\partial_l = \partial/\partial y^l$ and $\partial_{l'} = \partial/\partial y^{l'}$ satisfy the relations

$$\partial_l = \tfrac{1}{2}\partial^{l'}, \quad \partial_{l'} = \tfrac{1}{2}\partial^l, \quad l = 1,...,\nu.$$

We have the following proposition.

Proposition 2.1: The Dirac equation (2.6) is equivalent to the following set of equations:

$$2q\partial_{[i_1}\psi_{i_2 i_3 \cdots i_q]} + \sum_{i_{q+1}=1}^{\nu} \partial^{i_{q+1}}\psi_{i_1 \cdots i_q i_{q+1}} = 0,$$

$$q = 1,3,5,...,2[(\nu-1)/2] + 1. \tag{2.7}$$

(We make the convention $\psi_{i_1 \cdots i_\rho} \equiv 0$, for $\rho > \nu$.)

Proof: From Eqs. (2.8a) and (2.8b) of Ref. 3, we have

$$\begin{aligned} &\sum_{l=1}^{\nu}(H_l\partial^l\psi)_{i_1 \cdots i_q} \\ &= \sum_{i_{q+1}=1}^{\nu}(H_{i_{q+1}})_{i_1 \cdots i_q}{}^{i_1 \cdots i_q i_{q+1}}\partial^{i_{q+1}}\psi_{i_1 \cdots i_q i_{q+1}} \\ &= \sum_{i_{q+1}=1}^{\nu}\partial^{i_{q+1}}\psi_{i_1 \cdots i_q i_{q+1}}, \end{aligned} \tag{2.8}$$

and

$$\begin{aligned} &\sum_{l=1}^{\nu}(H_{l'}\partial^{l'}\psi)_{i_1 \cdots i_q} \\ &= \sum_{m=1}^{q}(H_{i'_m})_{i_1 \cdots i_q}{}^{i_1 \cdots \hat{i}_m \cdots i_q}\partial^{i'_m}\psi_{i_1 \cdots \hat{i}_m \cdots i_q} \\ &= \sum_{m=1}^{q}(-1)^{q-m}2\partial_{i_m}\psi_{i_1 \cdots \hat{i}_m \cdots i_q} \\ &= 2q\partial_{[i_1}\psi_{i_2 i_3 \cdots i_q]}. \end{aligned} \tag{2.9}$$

(A sign $\hat{}$ over an index means that that particular index is missing from the sequence in which it appears.) Inserting

Eqs. (2.8) and (2.9) into Eq. (2.6b) we get Eq. (2.7). ▼

The first two cases, i.e., $q = 1,3$, are given explicitly by the following two equations:

$$2\,\partial_{i_1}\psi_0 + \sum_{i_2=1}^{\nu} \partial^{i_2}\psi_{i_1 i_2} = 0, \tag{2.10}$$

and

$$6\,\partial_{[i_1}\psi_{i_2 i_3]} + \sum_{i_4=1}^{\nu} \partial^{i_4}\psi_{i_1 i_2 i_3 i_4} = 0. \tag{2.11}$$

We want to show now that the $\binom{\nu}{q}$ equations (2.7) are redundant for $q>5$. In fact we have the following proposition.

Proposition 2.2: If Eqs. (2.10) and (2.11) are satisfied, then for $q>5$ all remaining equations (2.7) are automatically satisfied.

Proof: The Dirac equation (2.7) for odd q can be written in the form

$$\binom{q}{3}\left\{6(\partial_{[i_1}\psi_{i_2 i_3]}) + \sum_{i_{q+1}=1}^{\nu} (\partial_{i_{q+1}}\psi_{[i_1 i_2 i_3}{}^{i_{q+1}})\right\}\psi_{i_4 \cdots i_q]}$$
$$+ \frac{q(3-q)}{2}\left\{2(\partial_{[i_1}\psi_0) + \sum_{i_{q+1}=1}^{\nu} (\partial_{i_{q+1}}\psi_{[i_1}{}^{i_{q+1}})\right\}$$
$$\times \psi_{i_2 \cdots i_q]} = 0. \tag{2.12}$$

In fact, using Eq. (A16), we have that

$$\partial_{[i_1}\psi_{i_2 \cdots i_q]}$$
$$= e^{-\alpha/2}\left\{\binom{q-1}{2}(\partial_{[i_1}\psi_{i_2 i_3)})\psi_{i_4 \cdots i_q]}\right.$$
$$\left. + \frac{1}{3}(3-q)(\partial_{[i_1}\psi_0)\psi_{i_2 \cdots i_q]}\right\}, \tag{2.13}$$

while, using Eqs. (A16), (A1), and (A2) we have that

$$\partial_{i_{q+1}}\psi_{i_1 \cdots i_q}{}^{i_{q+1}}$$
$$= e^{-\alpha/2}\left\{\binom{q}{3}(\partial_{i_{q+1}}\psi_{[i_1 i_2 i_3}{}^{i_{q+1}})\psi_{i_4 \cdots i_q]}\right.$$
$$\left. + \frac{1}{2}q(3-q)(\partial_{i_{q+1}}\psi_{[i_1}{}^{i_{q+1}})\psi_{i_2 \cdots i_q]}\right\}. \tag{2.14}$$

After insertion of Eqs. (2.13) and (2.14) into Eq. (2.7) we obtain Eq. (2.12). Looking at Eq. (2.7) in the form given by Eq. (2.12) we see that, if Eqs. (2.10) and (2.11) are satisfied, then the expressions within the braces of Eq. (2.12) are identically zero, making Eq. (2.12) automatically satisfied in this way. ▼

We see therefore that the independent set of equations for a pure spinor field $\psi(x)$ is given by Eqs. (2.10) and (2.11). Since by Eq. (2.4)

$$\psi_{i_1 i_2 i_3 i_4} = 3\psi_0^{-1}\psi_{[i_1 i_2}\psi_{i_3 i_4]}, \tag{2.15}$$

the set of equations (2.10) and (2.11) represents, in fact, a set of nonlinear equations for ψ_0 and $\psi_{i_1 i_2}$ with a highly nontrivial *nonpolynomial* nonlinearity given by Eq. (2.15).

We shall show now that, using the $[1 + \binom{\nu}{2}]$ spinor coordinates, we can reduce Eqs. (2.10) and (2.11) to a system of nonlinear equations with quadratic nonlinearities. We recall that in the considered representation, the highest weight spinor ψ_{m_+} for the highest weight $m_+ = (\frac{1}{2},\ldots,\frac{1}{2})$ can be written in the form

$$\psi_{m_+} = \left|\left|\begin{matrix}1\\0\\\vdots\\0\end{matrix}\right|\right|. \tag{2.16}$$

As follows from the Cartan theory, the space of all pure semispinors associated with m_+ is given by the formula[6]

$$\psi = T_g\psi_{m_+}, \tag{2.17}$$

where $g \to T_g$ is the $SO(\nu,\nu)$ spinor representation. We showed in Ref. 3 that ψ_{m_+} has the stability group

$$H = SL(\nu,\mathbb{R}) \circledS T^{\binom{\nu}{2}},$$

where $T^{\binom{\nu}{2}}$ is an Abelian group of dimension $\binom{\nu}{2}$. According to the Mackey decomposition theorem,[8] there exists a Borel set $C \subset SO(\nu,\nu)$ such that any $g \in SO(\nu,\nu)$ has the decomposition

$$g = ch, \quad c \in C, \quad h \in H.$$

Then the pure spinor (2.17) can be written in the form

$$\psi = T_c\psi_{m_+} = \psi(c),$$

i.e., the elements of the pure spinor space can be parametrized by the elements c of the set C. We have shown in Ref. 3, the remarkable fact that in the case of the $SO(\nu,\nu)$ group the set C can be identified—up to a set of Haar measure zero—with the group space $T^{\binom{\nu}{2}} \circledS T^1$, i.e.,

$$C = T^{\binom{\nu}{2}} \circledS T^1.$$

Hence the group parameters $\{c_k\}_{k=1}^{1+\binom{\nu}{2}}$ may be considered as $[1 + \binom{\nu}{2}]$ intrinsic coordinates of the pure semispinor $\psi(c)$.

The action of T_{g_0} on $\psi(c)$ is determined by the Mackey decomposition; in fact

$$T_{g_0}\psi(c) = T_{g_0 c}\psi_{m_+} = \psi(c_{g_0 c}),$$

where the group element $c_{g_0 c}$ is uniquely determined by the formula

$$g_0 c = c_{g_0 c}h_{g_0 c}.$$

We see that if we represent ψ in terms of $\{c_k\}_{k=1}^{1+\binom{\nu}{2}}$, the action of $SO(\nu,\nu)$ on ψ is nonlinear.

It is shown in Ref. 7 that we can choose a parametrization of the group G such that it is expressed as a product of one-parameter subgroups, i.e.,

$$e^{\tilde{X}} = \left[\prod_{k<l=1}^{\nu} \exp(c_{kl}\tilde{Q}^{kl})\right] e^{\alpha\tilde{D}},$$

where the $\tilde{Q}^{kl}$ are generators of $T^{\binom{\nu}{2}}$ and $\tilde{D}$ of T^1 groups, respectively. Then the generic non-null component of ψ, with an even number $2p$ of indices, is given by[7]

$$\psi_{i_1 \cdots i_{2p}} = (2p-1)!!e^{\alpha/2}c_{[i_1 i_2}c_{i_3 i_4} \cdots c_{i_{2p-1} i_{2p}]}; \tag{2.18}$$

Inserting (2.18) into (2.10) and (2.11), we get

$$\partial_{i_1}\alpha + \sum_{i_2=1}^{\nu}\left[\partial^{i_2}c_{i_1 i_2} + \frac{1}{2}c_{i_1 i_2}\partial^{i_2}\alpha\right] = 0 \tag{2.19}$$

and

$$2\,\partial_{[i_1}c_{i_2 i_3]} + \sum_{i_4=1}^{\nu}(\partial^{i_4}c_{[i_1 i_2})c_{i_3]i_4} = 0, \tag{2.20}$$

with $i_1, i_2, i_3 = 1,\ldots,\nu$.

It seems noteworthy that spinors that carry out a nonlinear spinor representation associated with the highest weight m_+, satisfy—in intrinsic spinor coordinates—a specific system of nonlinear equations with quadratic nonlinearities. Thus nonlinear representations imply some specific nonlinear dynamics.

Equations (2.19) and (2.20) were obtained independently in Ref. 9 using the Chevalley formalism.

III. COVARIANT WAVE EQUATIONS FOR SO(ν + 1,ν) PURE SPINORS

Following Cartan[6] we pass from the orthonormal basis of the pseudo-Euclidean space $\mathbb{R}^{\nu+1,\nu}$ to the isotropic basis using the transformation

$$r' = \begin{Vmatrix} 0 & 0 & 1 \\ \frac{1}{2}\mathbf{1}_\nu & \frac{1}{2}\mathbf{1}_\nu & 0 \\ \frac{1}{2}\mathbf{1}_\nu & -\frac{1}{2}\mathbf{1}_\nu & 0 \end{Vmatrix}.$$

The new metric tensor $\tilde{g}'_{rs}$ has the form

$$\{\tilde{g}'_{rs}\} = \begin{Vmatrix} 1 & 0 & 0 \\ 0 & 0 & \frac{1}{2}\mathbf{1}_\nu \\ 0 & \frac{1}{2}\mathbf{1}_\nu & 0 \end{Vmatrix}.$$

The new coordinates in $\mathbb{R}^{\nu+1,\nu}$ are denoted by y^0, y^l, and $y^{l'}$ and the corresponding basis of the Clifford algebra by H_0, H_l, and $H_{l'}$, $l = 1,...,\nu$. The relation connecting the two bases are the same as in the SO(ν,ν) case, plus

$$y^0 = x^{2\nu+1} \quad \text{and} \quad H_0 = \Gamma_{2\nu+1}.$$

The Dirac equation (2.5) in y-coordinates has the form

$$\left[H_0 \frac{\partial}{\partial y_0} + \sum_{l=1}^{\nu} \left(H_l \frac{\partial}{\partial y_l} + H_{l'} \frac{\partial}{\partial y_{l'}}\right)\right] \psi(y) = 0. \tag{3.1}$$

The pure spinor ψ from the carrier space L^m of the irreducible linear representation of SO($\nu+1,\nu$) of dimension 2^ν, corresponding to the highest weight $m = (\frac{1}{2},...,\frac{1}{2})$, can be represented as a column

$$\psi = \begin{Vmatrix} \psi_0 \\ \psi_1 \\ \vdots \\ \psi_\nu \\ \psi_{12} \\ \vdots \\ \psi_{\nu-1\,\nu} \\ \vdots \\ \psi_{i_1 \cdots i_\nu} \end{Vmatrix}.$$

The components $\psi_{i_1 \cdots i_r}$ for $r \geqslant 3$ can be expressed in terms of ψ_0, ψ_{i_1}, and $\psi_{i_1 i_2}$ by the formulas[6,7]

$$\psi_{i_1 \cdots i_{2p}} = (2p-1)!!\psi_0^{1-p}\psi_{[i_1 i_2}\psi_{i_3 i_4} \cdots \psi_{i_{2p-1} i_{2p}]} \tag{3.2a}$$

and

$$\psi_{i_1 \cdots i_{2p+1}} = (2p+1)!!\psi_0^{-p}\psi_{[i_1}\psi_{i_2 i_3} \cdots \psi_{i_{2p} i_{2p+1}]}. \tag{3.2b}$$

We have the following proposition.

Proposition 3.1: The Dirac equation (3.1), written for the spinor components, has the form

$$\partial_0 \psi_{i_1 \cdots i_r} - 2r\,\partial_{[i_1}\psi_{i_2 \cdots i_r]} + \sum_{i_{r+1}=1}^{\nu} \partial^{i_{r+1}}\psi_{i_{r+1} i_1 \cdots i_r} = 0, \quad r = 0,1,2,...,\nu. \tag{3.3}$$

Proof: From Eqs. (2.8a)–(2.8c) of Ref. 3, we have

$$(H_0\,\partial_0\psi)_{i_1 \cdots i_r} = (-1)^r \partial_0 \psi_{i_1 \cdots i_r}, \tag{3.4}$$

$$\sum_{l=1}^{\nu} (H_l\,\partial^l\psi)_{i_1 \cdots i_r} = \sum_{i_{r+1}=1}^{\nu} (H_{i_{r+1}})_{i_1 \cdots i_r}{}^{i_1 \cdots i_r i_{r+1}}\,\partial^{i_{r+1}}\psi_{i_1 \cdots i_r i_{r+1}} = (-1)^r \sum_{i_{r+1}=1}^{\nu} \partial^{i_{r+1}}\psi_{i_{r+1} i_1 \cdots i_r}, \tag{3.5}$$

and

$$\sum_{l=1}^{\nu} (H_{l'}\,\partial^{l'}\psi)_{i_1 \cdots i_r} = \sum_{m=1}^{r} (H_{i'_m})_{i_1 \cdots i_r}{}^{i_1 \cdots \hat{i}_m \cdots i_r}\,\partial^{i'_m}\psi_{i_1 \cdots \hat{i}_m \cdots i_r} = \sum_{m=1}^{r} (-1)^{r-m} 2\,\partial_{i_m}\psi_{i_1 \cdots \hat{i}_m \cdots i_r} = (-1)^{r+1} 2r\,\partial_{[i_1}\psi_{i_2 \cdots i_r]}. \tag{3.6}$$

Inserting Eqs. (3.4) and (3.6) into Eq. (3.1) we obtain Eq. (3.3). ▼

The first $r = 0,1,2,3$ cases are given explicitly by the following equations:

$$\partial_0\psi_0 + \sum_{i_1=1}^{\nu} \partial^{i_1}\psi_{i_1} = 0, \tag{3.7}$$

$$\partial_0\psi_{i_1} - 2\,\partial_{i_1}\psi_0 - \sum_{i_2=1}^{\nu} \partial^{i_2}\psi_{i_1 i_2} = 0, \tag{3.8}$$

$$\partial_0\psi_{i_1 i_2} - 4\,\partial_{[i_1}\psi_{i_2]} + \sum_{i_3=1}^{\nu} \partial^{i_3}\psi_{i_1 i_2 i_3} = 0, \tag{3.9}$$

$$\partial_0\psi_{i_1 i_2 i_3} - 6\,\partial_{[i_1}\psi_{i_2 i_3]} - \sum_{i_4=1}^{\nu} \partial^{i_4}\psi_{i_1 i_2 i_3 i_4} = 0. \tag{3.10}$$

We show now that all equations in (3.3) for $r \geqslant 5$ follow from Eqs. (3.7)–(3.10). In fact, we have the following proposition.

Proposition 3.2: If the spinor components satisfy Eqs. (3.7)–(3.10), then they automatically satisfy all Eqs. (3.3) for any r.

Proof: For $r = q$ *odd* the Dirac equation (3.3) for the pure spinor components can be written as

$$\frac{1}{2}q(3-q)\left\{(\partial_0\psi_{[i_1}) - 2(\partial_{[i_1}\psi_0) - \sum_{i_{q+1}=1}^{\nu} (\partial_{i_{q+1}}\psi_{[i_1}{}^{i_{q+1}})\right\}\psi_{i_2 \cdots i_q]} + \left\{(\partial_0\psi_{[i_1 i_2 i_3}) - 6(\partial_{[i_1}\psi_{i_2 i_3}) - \sum_{i_{q+1}=1}^{\nu} (\partial_{i_{q+1}}\psi_{[i_1 i_2 i_3}{}^{i_{q+1}})\right\}\psi_{i_4 \cdots i_q]} = 0, \tag{3.11}$$

while for $r=p$ *even*, it can be written as

$$\left(1-\frac{p}{2}\right)\left\{\partial_0\psi_0+\sum_{i_{p+1}=1}^{\nu}(\partial_{i_{p+1}}\psi^{i_{p+1}})\right\}\psi_{i_1\cdots i_p}-\frac{1}{2}p(p-2)\left\{\partial_0\psi_{[i_1}-2\,\partial_{[i_1}\psi_0-\sum_{i_{p+1}=1}^{\nu}(\partial_{i_{p+1}}\psi_{[i_1}{}^{i_{p+1}})\right\}\psi_{i_2\cdots i_p]}$$
$$+\binom{p}{2}\left\{\partial_0\psi_{[i_1i_2}-4\,\partial_{[i_1}\psi_{i_2}+\sum_{i_{p+1}=1}^{\nu}(\partial_{i_{p+1}}\psi_{[i_1i_2}{}^{i_{p+1}})\right\}\psi_{i_2\cdots i_p]}$$
$$+\binom{p}{3}\left\{\partial_0\psi_{[i_1i_2i_3}-6\,\partial_{[i_1}\psi_{i_2i_3}-\sum_{i_{p+1}=1}^{\nu}(\partial_{i_{p+1}}\psi_{[i_1i_2i_3}{}^{i_{p+1}})\right\}\psi_{i_4\cdots i_p]}=0. \tag{3.12}$$

In fact from Eqs. (A6)–(A8), using Eqs. (A2), (3.7), and (3.9), we have that

$$\partial_0\psi_{i_1\cdots i_q}=e^{-\alpha/2}\left\{\frac{1}{2}q(3-q)(\partial_0\psi_{[i_1})\psi_{i_2\cdots i_q]}+\binom{q}{3}(\partial_0\psi_{[i_1i_2i_3})\psi_{i_4\cdots i_q]}\right\}, \tag{3.13}$$

while from Eq. (A16), we have that

$$q\partial_{[i_1}\psi_{i_2\cdots i_q]}=e^{-\alpha/2}\left[\binom{q}{3}3(\partial_{[i_1}\psi_{i_2i_3})\psi_{i_4\cdots i_q]}+\frac{1}{2}q(3-q)\,(\partial_{[i_1}\psi_0)\psi_{i_2\cdots i_q]}\right]. \tag{3.14}$$

After insertion of Eqs. (3.13), (3.14), and (2.14) into Eq. (3.3) for $r=q$ (odd), the first part of Proposition 3.2 is proved.

Let us pass to the case $r=p$ even. From Eq. (A16), we have that

$$\partial_0\psi_{i_1\cdots i_p}=e^{-\alpha/2}\left[\binom{p}{2}(\partial_0\psi_{[i_1i_2})\psi_{i_3\cdots i_p]}+\left(1-\frac{p}{2}\right)(\partial_0\psi_0)\psi_{i_1\cdots i_p}\right], \tag{3.15}$$

while from Eqs. (A6), (A7), and (A8), we have that

$$\partial_{[i_1}\psi_{i_2\cdots i_p]}=e^{-\alpha/2}\left\{(p-1)(\partial_{[i_1}\psi_{i_2})\psi_{i_3\cdots i_p]}+\binom{p-1}{2}(\partial_{[i_1}\psi_{i_2i_3})\psi_{i_4\cdots i_p]}+\left(1-\frac{p}{2}\right)(\partial_{[i_1}\psi_0)\psi_{i_2\cdots i_p]}\right\}. \tag{3.16}$$

Finally from Eqs. (A11), (A2), (A16), (A6), (A7), (A17), and (A14), we have that

$$\partial^{i_{p+1}}\psi_{i_1\cdots i_pi_{p+1}}=e^{-\alpha/2}\left\{\left(1-\frac{p}{2}\right)(\partial_{i_{p+1}}\psi^{i_{p+1}})\psi_{i_1\cdots i_p}+\frac{1}{2}p(p-2)(\partial_{i_{p+1}}\psi_{[i_1}{}^{i_{p+1}})\psi_{i_2\cdots i_p]}\right.$$
$$\left.+\binom{p}{2}(\partial_{i_{p+1}}\psi_{[i_1i_2}{}^{i_{p+1}})\psi_{i_3\cdots i_p]}-\binom{p}{3}(\partial_{i_{p+1}}\psi_{[i_1i_2i_3}{}^{i_{p+1}})\psi_{i_4\cdots i_p]}\right\}. \tag{3.17}$$

After insertion of Eqs. (3.15)–(3.17) into Eq. (3.3) for $r=p$ (even) and taking into account the relation (A18) also, Eqs. (3.11) and (3.12) are obtained.

Looking at Eq. (3.3) in the form given by Eqs. (3.11) and (3.12), we see that, if Eqs. (3.7)–(3.10) are satisfied, then the expressions within the braces of Eqs. (3.11) and (3.12) are identically zero, making Eq. (3.3) automatically satisfied. ▼

We see, therefore, that Eqs. (3.7)–(3.10) form a set of basic equations for the spinor ψ. Inserting Eqs. (3.2a) and (3.2b) for $\psi_{i_1i_2i_3}$ and $\psi_{i_1i_2i_3i_4}$ into (3.9) and (3.10), respectively, we see that the set (3.7)–(3.10) represents for the independent components ψ_0, ψ_{i_1}, and $\psi_{i_1i_2}$ a system of nonlinear equations with nonpolynomial nonlinearities.

We show now that, passing to the intrinsic spinor components, determined by the coordinates $\{c_k\}_{k=1}^{1+\binom{\nu+1}{2}}$ of the Mackey set C, we reduce the Eqs. (3.7)–(3.10) to a system of equations with quadratic nonlinearities. We note first that the highest weight spinor ψ_m, corresponding to the highest weight $m=(\frac{1}{2},\ldots,\frac{1}{2})$ of the $SO(\nu+1,\nu)$ spinor representation, still has the form (2.16). We have shown in Ref. 3 that the stability group H of ψ_m has the form

$$H=SL(\nu,\mathbf{R})\circledS\tilde{R},$$

where $\tilde{R}$ is a solvable Lie group whose Lie algebra $\tilde{r}$ has the form

$$\tilde{r}=t^{\binom{\nu}{2}}+d^{\nu},$$

with $t^{\binom{\nu}{2}}$ a $\binom{\nu}{2}$-dimensional Abelian algebra and d^{ν} a ν-dimensional vector space in the $so(\nu+1,\nu)$ Lie algebra. The corresponding set C coincides—up to a set of Haar measure zero—with the group space

$$C=R^{1}\circledS R, \tag{3.18}$$

where R is a solvable Lie group whose Lie algebra r has the following structure:

$$r=t^{\binom{\nu}{2}}+f^{\nu}, \tag{3.19}$$

with $t^{\binom{\nu}{2}}$ a $\binom{\nu}{2}$-dimensional Abelian Lie algebra and f^{ν} a ν-dimensional vector space in the $so(\nu+1,\nu)$ Lie algebra. We see that now the structure of the set C is much richer than in the $SO(\nu,\nu)$ case.

Since $g=ch$, $c\in C$, $h\in H$, then the arbitrary pure spinor ψ in the carrier space of the nonlinear representation can be written in the form

$$\psi=T_c\psi_m=\psi(c). \tag{3.20}$$

Consequently the group parameters of C may be considered

as the intrinsic components of ψ. We have shown in Ref. 7 that if $\tilde{F}^k$ and $\tilde{Q}^{rs}$ are generators of one-parameter subgroups in the space $t^{(\nu)}$ and f^{ν}, respectively, then for $\tilde{X} = g_k \tilde{F}^k + d_{rs}\tilde{Q}^{rs}$ in r, the representation $T_c = e^{\tilde{X}}$ can be written in the form

$$e^{\tilde{X}} = \left[\prod_{k=1}^{\nu} \exp(g_k \tilde{F}^k)\right]\left[\prod_{r<s=1}^{\nu} \exp(\tilde{d}_{rs}\tilde{Q}^{rs})\right] e^{\alpha \tilde{D}}. \quad (3.21)$$

Then the components of ψ with an even number p of indices are given by[7]

$$\psi_{i_1 \cdots i_p} = (p-1)!! e^{\alpha/2} d_{[i_1 i_2} d_{i_3 i_4} \cdots d_{i_{p-1} i_p]}, \quad (3.22)$$

while those ones with an odd number q of indices are given by[7]

$$\psi_{i_1 \cdots i_q} = -q!! e^{\alpha/2} g_{[i_1} d_{i_2 i_3} \cdots d_{i_{q-1} i_q]}, \quad (3.23)$$

where

$$d_{ij} := \tilde{d}_{ij} + \epsilon(j-i) g_i g_j. \quad (3.24)$$

Inserting formulas (3.22)–(3.24) into Eqs. (3.7)–(3.10), we find that the Dirac equation for the pure spinor $\psi(y)$ transforms into the following set of nonlinear equations for the intrinsic spinor coordinates $\alpha(y)$, $g_i(y)$, and $d_{jk}(y)$:

$$\frac{1}{2}\partial_0 \alpha - \sum_{i_1=1}^{\nu}\left(\frac{1}{2} g_{i_1}\partial^{i_1}\alpha + \partial^{i_1} g_{i_1}\right) = 0, \quad (3.25)$$

$$\tfrac{1}{2}(\partial_0 \alpha) g_{i_1} + \partial_0 g_{i_1} + \partial_{i_1}\alpha + \sum_{i_2=1}^{\nu}\left(\frac{1}{2} d_{i_1 i_2}\partial^{i_2}\alpha + \partial^{i_2} d_{i_1 i_2}\right) = 0, \quad (3.26)$$

$$\tfrac{1}{2}\partial_0 d_{i_1 i_2} + g_{[i_1}\partial_0 g_{i_2]} + 2\partial_{[i_1} g_{i_2]} - \sum_{i_3=1}^{\nu}\left[(\partial^{i_3} g_{[i_1}) d_{i_2]i_3} + \frac{1}{2} g_{i_3}\partial^{i_3} d_{i_1 i_2}\right] = 0, \quad (3.27)$$

$$g_{[i_1}\partial_0 d_{i_2 i_3]} + 2\partial_{[i_1} d_{i_2 i_3]} + \sum_{i_4=1}^{\nu}(\partial^{i_4} d_{[i_1 i_2}) d_{i_3]i_4} = 0. \quad (3.28)$$

We see that in intrinsic spinor coordinates, provided by the group parameters of the C group, the Dirac equation (2.5) represents a system of specific nonlinear first-order equations with quadratic nonlinearities. Due to the more complex structure of the C space, the system (3.25)–(3.28) of nonlinear equations is also much more complicated than the corresponding system (2.19) and (2.20) for the SO(ν,ν) case.

IV. PARTIALLY PURE SPINORS

The theory presented in Secs. II and III concerns the nonlinear wave equations associated with pure spinors of SO(ν,ν) and SO($\nu+1,\nu$) groups. We would like to call attention to a rather interesting fact that the pure spinor representation of the given rotation group represents one out of, in general, many nonlinear spinor representations. Consider the case of the SO($\nu+1,\nu$) groups. In this case the carrier spinor space L^m of the linear spinor representation is spanned by the spinors

$$\psi = \begin{Vmatrix} \psi_0 \\ \vdots \\ \psi_{i_1} \\ \vdots \\ \psi_{i_1 i_2} \\ \vdots \\ \psi_{i_1 \cdots i_\nu} \end{Vmatrix} \quad (4.1)$$

and has dimension $d_\psi = 2^\nu$. In the case of the pure spinor ψ_p the components $\psi_{i_1 \cdots i_p}$ are determined by the ψ_0, ψ_{i_1}, and $\psi_{i_1 i_2}$ components, in particular by Eq. (3.2),

$$\psi_{12\cdots\nu} = \begin{cases} (\nu-1)!! \psi_0^{1-\nu/2}\psi_{[12}\psi_{34}\cdots\psi_{\nu-1\nu]}, \\ \qquad \text{for } \nu \text{ even}, \\ \nu!! \psi_0^{(1-\nu)/2}\psi_{[1}\psi_{23}\cdots\psi_{\nu-1\nu]}, \\ \qquad \text{for } \nu \text{ odd} \end{cases}$$

must be zero for any pure spinor having all $\psi_{i_1 i_2}$ components zero, like the standard pure spinor $\overset{1}{\psi}_m$ given by Eq. (1.3). Hence the spinor

$$\overset{2}{\psi}_m := \begin{Vmatrix} 1 \\ 0 \\ \vdots \\ 0 \\ 1 \end{Vmatrix} \quad (4.2)$$

is certainly *not* pure. Consequently the nonlinear spinor representation determined by $\overset{2}{\psi}_m$, according to the construction given in Sec. III will be different from that associated with the pure spinor $\overset{1}{\psi}_m$. In order to find this representation one has to determine the stability group $\overset{2}{H}$ of $\overset{2}{\psi}_m$ and the Mackey set $\overset{2}{C} = \mathrm{SO}(\nu+1,\nu)/\overset{2}{H}$. We have the following theorem.

Theorem 4.1: Let $m = (\frac{1}{2},\ldots,\frac{1}{2})$ be the highest weight of the irreducible linear spinor representation of the SO($\nu+1,\nu$) group with $\nu \geqslant 5$. Then the stability group $\overset{2}{H}$ of $\overset{2}{\psi}_m$ is the group SL($\nu,\mathbb{R}$) spanned by the (ν^2-1) generators

$$\Pi^{kl} = -\frac{1}{2}[H_k, H_{l'}] + \frac{\delta_{kl}}{\nu}\sum_{m=1}^{\nu}\frac{1}{2}[H_m, H_{m'}], \quad k,l = 1,\ldots,\nu. \quad (4.3)$$

Proof: (See Appendix B.)

Remark: Contrary to the pure case, here the set of generators in so($\nu+1,\nu$), complementary to the stability set $\{\Pi^{kl}\}$, do not form an algebra.

Notice that in the case of the standard pure spinor $\overset{1}{\psi}_m$ the stability group was the group

$$\overset{1}{H} = R \circledS \mathrm{SL}(\nu,\mathbb{R}),$$

where R is a solvable group whose Lie algebra r has the following structure[3]:

$$r = t^{(\nu_2)} \dot{+} d^{\nu},$$

with $t^{(\nu_2)}$ a $\binom{\nu}{2}$-dimensional Abelian Lie algebra and d^{ν} a ν-dimensional vector space in the so$(\nu+1,\nu)$ Lie algebra. We see therefore that $\overset{2}{H}$ coincides with the maximal simple subgroup of $\overset{1}{H}$.

The Mackey set $\overset{2}{C} = \mathrm{SO}(\nu+1,\nu)/\overset{2}{H}$ has the dimension $d_{\underset{C}{2}} = 1 + 2\nu + 2\binom{\nu}{2}$, which is much larger than the dimension $d_{\underset{C}{1}} = 1 + \nu + \binom{\nu}{2}$ of $\overset{1}{C}$ in the pure spinor case. It follows from the form of $\overset{1}{\psi}_m$ that the pure spinor is distinguished by the fact that the dimension of the associated nonlinear spinor representation is the highest one.

As previously, the carrier space $\overset{2}{N}{}^m$ of the nonlinear spinor representation associated with $\overset{2}{\psi}_m$ coincides with the manifold $\overset{2}{C}$, i.e.,

$$\overset{2}{\psi}(c) = \overset{2}{T}_c \overset{2}{\psi}_m, \quad c \in \overset{2}{C}.$$

The nonlinear representation $\overset{2}{T}$ acts in $\overset{2}{N}{}^m$ according to the formula

$$\overset{2}{T}_{g_0} \overset{2}{\psi}(c) = \overset{2}{\psi}(c_{g_0 c}).$$

It is clear that, taking another standard spinor $\overset{3}{\psi}_m$ with a larger-than-2 number of nonvanishing components, one obtains in general a still smaller stability group $\overset{3}{H}$ and a larger carrier space $\overset{3}{N}{}^m \sim \overset{3}{C}$ of the nonlinear spinor representation $\overset{3}{T}$ of $\mathrm{SO}(\nu+1,\nu)$. In that manner, determining a finite number n of all nonequivalent stability subgroups $\overset{i}{H}$ of $\overset{i}{\psi}_m$, one finds all possible nonlinear spinor representations $\overset{i}{T}$, $i = 1,2,\ldots,n$, associated with a given linear irreducible spinor representation. The dimensions d_i of these nonlinear representations will satisfy the inequalities

$$1 + \nu + \binom{\nu}{2} \leqslant d_2 \leqslant d_3 \leqslant \cdots \leqslant d_m < 2^{\nu}.$$

We shall call the corresponding nonlinear spinors "partially pure spinors." They represent a natural extension of the original Cartan pure spinor and they have a rich geometric, topological, and group theoretic structure.[10] The theory of nonlinear spinor wave equations associated with partially pure spinors will be presented elsewhere.[11]

V. DISCUSSION

We conclude this work with the following remarks.

(1) It is remarkable that, with every nonlinear pure spinor representation of a rotation group, one can associate nonlinear covariant spinor wave equations with a specific type of bilinear nonlinearity. The obtained models of spinor field theory resemble the σ models of boson field theories based on homogeneous spaces of the rotation group.[5] The Lagrangian formalism and the corresponding conservation laws of the obtained nonlinear spinor field theory are considered in Ref. 11. We stress that the resulting spinor field theory—due to a large number of bilinear constraints—contains an absolutely minimal number of independent spinor field components: for instance in the case of the $\mathrm{SO}(\nu+1,\nu)$ groups for $\nu = 10$, instead of 1024 independent spinor components in the linear representation, we have only 56 in the nonlinear one.

(2) The covariant form (2.6a) of the spinor wave equation is very convenient for coupling the spinor field ψ with other fields, e.g., gauge fields A_{μ}^{b} connected with a gauge group G. In fact in this case the coupled covariant wave equation will have the form

$$D_a(A)\Gamma^a \psi(x) = 0, \tag{5.1}$$

where

$$[D_a(A)]_{mn} = \delta_{mn} \frac{\partial}{\partial x^a} - ig(T^r)_{mn} A^r_a,$$

with $a = 1,\ldots,2\nu$ (or $2\nu+1$) and $m,n,r = 1,\ldots,\dim G$.

The analysis of the coupling of pure spinor fields with gauge fields may clarify the physical meaning of constrained spinor field theories.

(3) A systematic program of a quantization of a field theory with field values on homogeneous spaces has been considered in Refs. 12 and 13. This theory can be applied in our case and will provide a specific model of nonlinear spinor field theory with bilinear constraints. It is interesting that a model of spinor field theory with bilinear spinor constraints appears in the strong coupling limit of boson–fermion field theories.

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APPENDIX A: LEMMAS NEEDED IN THE PROOFS OF PROPOSITIONS 2.2 and 3.2

We collect here a series of results of technical nature.

Lemma 1: For *p even* we have

$$\psi_0 \psi_{i_1 \cdots i_p} = (p-1)\psi_{[i_1 \cdots i_{p-2}} \psi_{i_{p-1}] i_p}, \tag{A1}$$

and

$$\psi_0 \psi_{i_1 \cdots i_p} = (p-1)\psi_{[i_1 i_2} \psi_{i_3 \cdots i_p]}. \tag{A2}$$

Proof: From Ref. 6 we have that

$$\psi_0\psi_{i_1\cdots i_p}=\sum_{m=1}^{p-1}(-1)^{m-1}\psi_{i_m i_p}\psi_{i_1\cdots\hat{i}_m\cdots i_{p-1}}, \tag{A3}$$

which, after insertion of the definition (2.6), gives Eq. (A1).

In order to demonstrate Eq. (A2), let us write Eq. (2.4) explicitly, using definition (2.5)

$$\begin{aligned}\psi_0\psi_{i_1\cdots i_p}&=\frac{\psi_0^{1-(p/2-1)}}{p\cdot(p-2)!!}\Big\{(\psi_{i_1i_2}-\psi_{i_2i_1})\Big(\sum_{\pi(i_3,\ldots,i_p)}(-1)^{\pi}\psi_{i_{\pi_3}i_{\pi_4}}\cdots\psi_{i_{\pi_{p-1}}i_{\pi_p}}\Big)\\&\quad+\cdots+(\psi_{i_{p-1}i_p}-\psi_{i_pi_{p-1}})\Big(\sum_{\pi(i_1,\ldots,i_{p-2})}(-1)^{\pi}\psi_{i_{\pi_1}i_{\pi_2}}\cdots\psi_{i_{\pi_{p-3}}i_{\pi_{p-2}}}\Big)\Big\}\\&=\frac{1}{p}\{(\psi_{i_1i_2}-\psi_{i_2i_1})\psi_{i_3i_4,\ldots,i_p}+\cdots+(\psi_{i_{p-1}i_p}-\psi_{i_pi_{p-1}})\psi_{i_1i_2\cdots i_{p-2}}\},\end{aligned} \tag{A4}$$

while, using definition (2.5) again,

$$\begin{aligned}\psi_{[i_1i_2}\psi_{i_3\cdots i_p]}&=\frac{1}{p!}\{(\psi_{i_1i_2}-\psi_{i_2i_1})(\psi_{i_3\cdots i_p}+\text{perm})\\&\quad+\cdots+(\psi_{i_{p-1}i_p}-\psi_{i_pi_{p-1}})(\psi_{i_1\cdots i_{p-2}}+\text{perm})\}\\&=\frac{1}{p(p-1)}\{(\psi_{i_1i_2}-\psi_{i_2i_1})\psi_{i_3\cdots i_p}\\&\quad+\cdots+(\psi_{i_{p-1}i_p}-\psi_{i_pi_{p-1}})\psi_{i_1\cdots i_{p-2}}\}.\end{aligned} \tag{A5}$$

Comparing Eqs. (A4) and (A5), Eq. (A2) is proved. ▼

Lemma 2: For *q odd* we have

$$\psi_0\psi_{i_1\cdots i_q}=q\psi_{[i_1}\psi_{i_2\cdots i_q]}, \tag{A6}$$

$$\psi_0\psi_{i_1\cdots i_q}=q\psi_{[i_1i_2}\psi_{i_3\cdots i_q]}, \tag{A7}$$

$$\psi_0\psi_{i_1\cdots i_q}=\tfrac{1}{3}q(q-2)\psi_{[i_1i_2i_3}\psi_{i_4\cdots i_q]}. \tag{A8}$$

Proof: From Ref. 6 we have that

$$\psi_0\psi_{i_1\cdots i_q}=\sum_{m=1}^{q}(-1)^{m-1}\psi_{i_m}\psi_{i_1\cdots\hat{i}_m\cdots i_q}, \tag{A9}$$

which, using the definition (2.6), gives Eq. (A6). From Eqs. (A6) and (A2) we have

$$\begin{aligned}\psi_0^2\psi_{i_1\cdots i_q}&=q\psi_0\psi_{[i_1}\psi_{i_2\cdots i_q]}\\&=q(q-2)\psi_{[i_1}\psi_{i_2i_3}\psi_{i_4\cdots i_q]}\\&=q\psi_0\psi_{[i_1i_2}\psi_{i_3\cdots i_q]}\\&=q(q-2)\tfrac{1}{3}\psi_0\psi_{[i_1i_2i_3}\psi_{i_4\cdots i_q]},\end{aligned}$$

proving both Eq. (A7) and (A8). ▼

Lemma 3: For *q odd* we have

$$\psi_0\psi_{i_1\cdots i_{q+1}}=\tfrac{1}{3}q(q-2)\psi_{[i_1\cdots i_{q-3}}\psi_{i_{q-2}i_{q-1}i_q]i_{q+1}}. \tag{A10}$$

Proof: Applying Eqs. (A1) and (A2), we have

$$\begin{aligned}\psi_0^2\psi_{i_1\cdots i_{q+1}}&=q\psi_0\psi_{[i_1\cdots i_{q-1}}\psi_{i_q]i_{q+1}}\\&=q(q-2)\psi_{[i_1i_2}\psi_{i_3\cdots i_{q-1}}\psi_{i_q]i_{q+1}}\\&=\tfrac{1}{3}q(q-2)\psi_0\psi_{[i_1\cdots i_{q-3}}\psi_{i_{q-2}i_{q-1}i_q]i_{q+1}},\end{aligned}$$

and the lemma is proved. ▼

Lemma 4: For *p even* we have

$$\psi_0\psi_{i_1\cdots i_{p+1}}=p\psi_{[i_1}\psi_{i_2\cdots i_p]i_{p+1}}+\psi_{i_1\cdots i_p}\psi_{i_{p+1}}, \tag{A11}$$

$$\psi_0\psi_{i_1\cdots i_{p+1}}=p\psi_{[i_1\cdots i_{p-1}}\psi_{i_p]i_{p+1}}+\psi_{i_1\cdots i_p}\psi_{i_{p+1}}, \tag{A12}$$

$$\begin{aligned}\psi_0\psi_{i_1\cdots i_{p+1}}&=(p-1)\psi_{[i_1i_2}\psi_{i_3\cdots i_p]i_{p+1}}\\&\quad+2\psi_{[i_1\cdots i_{p-1}}\psi_{i_p]i_{p+1}},\end{aligned} \tag{A13}$$

$$\begin{aligned}\psi_0\psi_{i_1\cdots i_{p+1}}&=(p-1)\{\psi_{[i_1\cdots i_{p-2}}\psi_{i_{p-1}i_p]i_{p+1}}\\&\quad+\tfrac{1}{3}(p-2)\psi_{[i_1\cdots i_{p-3}}\psi_{i_{p-2}i_{p-1}i_p]i_{p+1}}\}.\end{aligned} \tag{A14}$$

Proof: From Eq. (A6) and definition (2.6) we have

$$\begin{aligned}\psi_0\psi_{i_1\cdots i_{p+1}}&=\psi_{i_1}\psi_{i_2\cdots i_{p+1}}-\psi_{i_2}\psi_{i_1\hat{i}_2\cdots i_{p+1}}\\&\quad+\cdots-\psi_{i_p}\psi_{i_1\cdots\hat{i}_pi_{p+1}}+\psi_{i_{p+1}}\psi_{i_1\cdots i_p}\\&=p\psi_{[i_1}\psi_{i_2\cdots i_p]i_{p+1}}+\psi_{i_{p+1}}\psi_{i_1\cdots i_p},\end{aligned}$$

and Eq. (A11) is proved. Using now Eq. (A1) and (A6) we may write

$$\begin{aligned}\psi_0\psi_{[i_1}\psi_{i_2\cdots i_p]i_{p+1}}&=(p-1)\psi_{[i_1}\psi_{i_2\cdots i_{p-1}}\psi_{i_p]i_{p+1}}\\&=\psi_0\psi_{[i_1\cdots i_{p-1}}\psi_{i_p]i_{p+1}}.\end{aligned} \tag{A15}$$

Inserting Eq. (A15) into Eq. (A11) we get Eq. (A12). Then from Eq. (A7) and definition (2.6) we have

$$\begin{aligned}\psi_0\psi_{i_1\cdots i_pi_{p+1}}&=(1/p!)\{[(\psi_{i_1i_2}\psi_{i_3\cdots i_pi_{p+1}}+\text{perm}(i_1,\ldots,i_p))-(\psi_{i_1i_2}\psi_{i_3\cdots i_{p-1}i_{p+1}i_p}+\text{perm}(i_1,\ldots,i_p))\\&\quad-\cdots-(\psi_{i_1i_2}\psi_{i_{p+1}i_4\cdots i_pi_3}+\text{perm}(i_1,\ldots,i_p))]-[(\psi_{i_1i_{p+1}}\psi_{i_3\cdots i_pi_2}+\text{perm}(i_1,\ldots,i_p))\\&\quad+(\psi_{i_{p+1}i_2}\psi_{i_3\cdots i_pi_1}+\text{perm}(i_1,\ldots,i_p))]\}\\&=(p-1)\psi_{[i_1i_2}\psi_{i_3\cdots i_p]i_{p+1}}-2\psi_{[i_1i_{p+1}}\psi_{i_2\cdots i_p]}\end{aligned}$$

(with i_{p+1} not antisymmetrized), and Eq. (A13) is proved. Finally, by repeated use of Eqs. (A13), (A2), and (A7) we have

$$\begin{aligned}\psi_0\psi_{i_1\cdots i_p}{}^{i_{p+1}} &= [(p-1)(p-3)/3]\psi_{[i_1i_2i_3i_4}\psi_{i_5\cdots i_p]}{}^{i_{p+1}} - 4\psi_{[i_1}{}^{i_{p+1}}\psi_{i_2\cdots i_p]} \\ &= (p-1)\psi_{[i_1\cdots i_{p-2}}\psi_{i_{p-1}i_p]}{}^{i_{p+1}} - (p-2)\psi_{[i_1}{}^{i_{p+1}}\psi_{i_2\cdots i_p]} \\ &= (p-1)\{\psi_{[i_1\cdots i_{p-2}}\psi_{i_{p-1}i_p]}{}^{i_{p+1}} - [(p-2)/3]\,\psi_{[i_1i_2i_3}{}^{i_{p+1}}\psi_{i_4\cdots i_p]}\},\end{aligned}$$

and Eq. (A14) also is proved. ▼

Lemma 5: For p *even* we have

$$\psi_0\partial^a\psi_{i_1\cdots i_p} = \binom{p}{2}(\partial^a\psi_{[i_1i_2})\psi_{i_3\cdots i_p]} + \left(1-\frac{p}{2}\right)(\partial^a\psi_0)\psi_{i_1\cdots i_p}. \tag{A16}$$

Proof: From Eqs. (A2) and (2.4) we have, acting recursively with the derivative,

$$\begin{aligned}\partial^a(\psi_0\psi_{i_1\cdots i_p}) &= (p-1)\{(\partial^a\psi_{[i_1i_2})\psi_{i_3\cdots i_p]} + \psi_0^{-1}\psi_{[i_1i_2}\partial^a(\psi_0\psi_{i_3\cdots i_p]}) - (\partial^a\psi_0)\psi_{i_1\cdots i_p}\} \\ &= \cdots = [(p-2)/2](p-1)(\partial^a\psi_{[i_1i_2})\psi_{i_3\cdots i_p]} + (p-1)!!\psi_0^{1-p/2}\psi_{[i_1i_2}\psi_{i_3i_4}\cdots\psi_{i_{p-3}i_{p-2}}\partial^a(\psi_0\psi_{i_{p-1}i_p]}) \\ &\quad - [(p-2)/2](\partial^a\psi_0)\psi_{i_1\cdots i_p} = \binom{p}{2}(\partial^a\psi_{[i_1i_2})\psi_{i_3\cdots i_p]} + \left(2-\frac{p}{2}\right)(\partial^a\psi_0)\psi_{i_1\cdots i_p},\end{aligned}$$

▼

and the lemma is proved.

Lemma 6: For q *odd* we have

$$\begin{aligned}&\psi_0\partial^a\psi_{i_1\cdots i_q} \\ &\quad = q(\partial^a\psi_{[i_1})\psi_{i_2\cdots i_q]} + \tbinom{q}{2}(\partial^a\psi_{[i_1i_2})\psi_{i_3\cdots i_q]} \\ &\qquad + \tfrac{1}{2}(1-q)(\partial^a\psi_0)\psi_{i_1\cdots i_q}.\end{aligned} \tag{A17}$$

Proof: Using Eqs. (A6) and (A16) we have

$$\begin{aligned}&\partial^a(\psi_0\psi_{i_1\cdots i_q}) \\ &\quad = q(\partial^a\psi_{[i_1})\psi_{i_2\cdots i_q]} + q\tbinom{q-1}{2}\psi_0^{-1}(\partial^a\psi_{[i_1i_2})\psi_{i_3}\psi_{i_4\cdots i_q]} \\ &\qquad + \tfrac{1}{2}(3-q)(\partial^a\psi_0)\psi_{i_1\cdots i_q}.\end{aligned}$$

Then, taking into account Eq. (A6), the lemma is proved. ▼

Lemma 7: For p *even* the following identity holds:

$$\frac{1}{2}p(p-2)(\partial^a\psi_{[i_1})\psi_{i_2\cdots i_p]} \equiv \binom{p}{3}(\partial^a\psi_{[i_1i_2i_3})\psi_{i_4\cdots i_p]}. \tag{A18}$$

Proof: From Eq. (A6) and (A8) we have

$$\begin{aligned}&-\tfrac{1}{2}p(p-2)(\partial^a\psi_{[i_1})\psi_{i_2\cdots i_p]} \\ &\quad + \tbinom{p}{3}(\partial^a\psi_{[i_1i_2i_3})\psi_{i_4\cdots i_p]} \\ &\quad = \tbinom{p}{3}(p-3)\psi_0^{-1}[\partial^a(\psi_{[i_1i_2i_3}\psi_{i_4})]\psi_{i_5\cdots i_p}\} \equiv 0.\end{aligned}$$

In fact from Eq. (A6) we have that

$$\psi_{[i_1i_2i_3}\psi_{i_4]} = 3\psi_0^{-1}\psi_{[i_1i_2}\psi_{i_3}\psi_{i_4]} \equiv 0,$$

and then the lemma is proved. ▼

APPENDIX B: PROOF OF THEOREM 4.1

Let us analyze the elements of the first and the last column of the matrices

$$\tfrac{1}{2}[H_\rho, H_\sigma], \quad \rho,\sigma = 0,1,\ldots,\nu,1',\ldots,\nu', \tag{B1}$$

making use of the Eqs. (2.8a)–(2.8c) of Ref. 3.

Then we have for the first column's elements

$$(\tfrac{1}{2}[H_j,H_0])_{i_1\cdots i_p}{}^0 = (\tfrac{1}{2}[H_j,H_l])_{i_1\cdots i_p}{}^0 = 0, \tag{B2a}$$

and

$$(\tfrac{1}{2}[H_j,H_0])_{i_1\cdots i_p}{}^0 = \delta_{p1}\delta_{i_1j}, \tag{B2b}$$

$$(\tfrac{1}{2}[H_f,H_{l'}])_{i_1\cdots i_p}{}^0 = \delta_{p2}(\delta_{i_1l}\delta_{i_2j} - \delta_{i_1j}\delta_{i_2l}), \tag{B2c}$$

$$(\tfrac{1}{2}[H_j,H_{l'}])_{i_1\cdots i_p}{}^0 = \delta_{p0}\tfrac{1}{2}\delta_{jl}. \tag{B2d}$$

For the last column we have

$$(\tfrac{1}{2}[H_f,H_0])_{i_1\cdots i_p}{}^{1\cdots\nu} = (\tfrac{1}{2}[H_f,H_{l'}])_{i_1\cdots i_p}{}^{1\cdots\nu} = 0, \tag{B3a}$$

while for the remaining ones the only non-null elements are given by

$$(\tfrac{1}{2}[H_j,H_0])_{1\cdots\hat{j}\cdots\nu}{}^{1\cdots\nu} = (-1)^j, \tag{B3b}$$

$$(\tfrac{1}{2}[H_j,H_l])_{1\cdots\hat{j}\cdots\hat{l}\cdots\nu}{}^{1\cdots\nu} = (-1)^{j+l+1}\epsilon(l-j), \tag{B3c}$$

$$(\tfrac{1}{2}[H_j,H_{l'}])_{1\cdots\nu}{}^{1\cdots\nu} = -\tfrac{1}{2}\delta_{jl}. \tag{B3d}$$

Summing up Eqs. (B2a)–(B3d), we have the following:

- $\frac{1}{2}[H_j,H_0]$ gives no contribution in the first column and a contribution $(-1)^j$ in the $(1\cdots\hat{j}\cdots\nu)$th row of the last column;
- $\frac{1}{2}[H_f,H_0]$ gives a contribution 1 in the jth row of the first column and no contribution in the last column;
- $\frac{1}{2}[H_j,H_l]$ gives no contribution in the first column and a contribution $(-1)^{j+l+1}\epsilon(l-j)$ in the $(1\cdots\hat{j}\cdots\hat{l}\cdots\nu)$th row of the last column;
- $\frac{1}{2}[H_f,H_{l'}]$ gives a contribution $\epsilon(j-l)$ in the (jl)th row of the first column and no contribution in the last column;
- $\frac{1}{2}[H_j,H_{l'}]$ for $j\neq l$ gives no contribution either in the first or in the last column;
- $\frac{1}{2}[H_j,H_f]$ gives a contribution $\frac{1}{2}$ in the 0th row of the first column and a contribution $(-\frac{1}{2})$ in the $(1\cdots\nu)$th row of the last column.

If we now go to the explicit realization of the $so(\nu+1,\nu)$ Lie algebra given by Eqs. (A2c), (A2d),

(A3c), (A3g), (C2), and (C3c) (for $h = \nu$), we see that the stability algebra of the spinor $\overset{2}{\psi}_m$, given by Eq. (4.2), is provided by the $\nu(\nu-1)$ generators $\frac{1}{2}[H_j, H_{l'}]$ with $j \neq l = 1,...,\nu$, plus $\nu - 1$ differences of generators $\frac{1}{2}[H_j, H_{j'}]$, $j = 1,...,\nu$, i.e., by the $(\nu^2 - 1)$ generators Π^{kl} given by Eq. (4.3). ▼

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Matrix operator symmetries of the Dirac equation and separation of variables

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The set of all matrix-valued first-order differential operators that commute with the Dirac equation in n-dimensional complex Euclidean space is computed. In four dimensions it is shown that all matrix-valued second-order differential operators that commute with the Dirac operator in four dimensions are obtained as products of first-order operators that commute with the Dirac operator. Finally some additional coordinate systems for which the Dirac equation in Minkowski space can be solved by separation of variables are presented. These new systems are comparable to the separation in oblate spheroidal coordinates discussed by Chandrasekhar [S. Chandrasekhar, *The Mathematical Theory of Black Holes* (Oxford U.P., Oxford, 1983)].

I. INTRODUCTION

A complete theory of separation of variables for the nonscalar equations of mathematical physics has yet to be developed. Some partial results have been obtained for the Dirac equation, the Proca equation, and the Pauli–Fierz equation.[1–3] More recently there has been renewed interest in the separability properties of the equations for first-order perturbations of spin fields in a gravitational background. In particular Teukolsky[4] has shown that for massless fields of spin-0, -½, and -1, a form of separable solution does exist for perturbations in a Kerr metric gravitational background. Chandrasekhar[5] has shown that the Dirac equation also admits a separable solution in such a background. These results have been extended by several authors[6,7] and shown to hold for more general classes of type D vacuum metrics. More recently the constant of the motion associated with the separation of variables for the Dirac equation (the other two constants are associated with geometrical symmetries) has been characterized.[8–10] It is found that the additional constant of the motion is a matrix first-order differential operator that commutes with the Dirac Hamiltonian. This operator is associated with the generalized Killing tensors of Yano and Bochner.[11] Furthermore McLenaghan and Spindel[9] have established the general form of a matrix first-order operator that commutes with the Dirac Hamiltonian. An interesting feature of Chandrasekhar's work is that it also implies that the Dirac equation in Minkowski space admits a separable solution in oblate spheroidal coordinates. We should mention in this connection the work of Cook[12] on separation of variables for the Dirac equation. These results inject new life into the possibility of classifying all separable coordinate systems and solutions for the Dirac equation. To this end in Sec. II we compute the matrix operators which commute with the Dirac Hamiltonian in complex Euclidean n-space. We then study the first- and second-order matrix symmetries of the Dirac equation in four dimensions in Sec. III culminating in Theorem I. Finally, in Sec. IV we present several examples of separable solutions (of the Dirac equation) in four-dimensional Minkowski space and give their operator characterization.

II. FIRST-ORDER CONSTANTS OF THE MOTION FOR THE DIRAC HAMILTONIAN IN E_n

In complex Euclidean n-space E_n Cartesian coordinates will be denoted by z_i, $i = 1,\ldots,n$, and the associated infinitesimal distance is

$$ds^2 = dz_i\, dz_i. \tag{2.1}$$

In this section repeated subscripts imply summation; we only use subscripts and work exclusively in Cartesian coordinates. Furthermore we will take the dimension to be $n = 2\nu$, i.e., even. Then, as is well known,[13] there is a unique representation of the Clifford algebra of dimension 2ν by $2\nu \times 2\nu$ matrices γ_i, which satisfy the anticommutation rules ($\{\ ,\ \}$ is the anticommutator bracket)

$$\{\gamma_i,\gamma_j\} = \gamma_i\gamma_j + \gamma_j\gamma_i = 2I_n\delta_{ij}. \tag{2.2}$$

The associated Dirac Hamiltonian is

$$H = \gamma_i\partial_i + m \quad \left(\partial_i = \frac{\partial}{\partial z_i}\right). \tag{2.3}$$

Clearly the results of significance in this section are to be obtained by considering various real forms of complex Euclidean n-space. The resulting Ψ, which is a solution of $H\Psi = 0$, could then be interpreted as the solution of an appropriate wave equation in a physical theory realized in dimension n. The other advantage of working in complex Euclidean n-space is that a large number of different cases for operators of a given type correspond to a single class in this case. The classification problem is thus made considerably simpler.

We now search for operators $L = F_a\,\partial_a + G$, which commute with H:

$$[H,L\,] = 0. \tag{2.4}$$

Equating to zero the coefficients of the derivatives in this condition we obtain

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$$[\gamma_a,F_b]+[\gamma_b,F_a]=0, \tag{2.5a}$$

$$[G,\gamma_a]=(\gamma_i\,\partial_i)F_a, \tag{2.5b}$$

$$(\gamma_i\,\partial_i)G=0. \tag{2.5c}$$

In addition to the γ_i matrices we define $\gamma_{2\nu+1}=\omega=(1/(2\nu)!)\,\epsilon_{i_1\cdots i_{2\nu}}\gamma_{i_1}\cdots\gamma_{i_{2\nu}}$. (Here $\epsilon_{i_1\cdots i_{2\nu}}$ is the usual antisymmetric tensor.) This matrix satisfies

$$\{\omega,\gamma_j\}=0 \quad j=1,\ldots,2\nu. \tag{2.6}$$

A suitable basis[13] for the space of $2\nu\times 2\nu$ matrices is then

$$\gamma_{a_1}\cdots\gamma_{a_{2p}},\quad p=1,\ldots,\nu,$$

$$\omega\gamma_{a_1}\cdots\gamma_{a_{2p-1}},\quad p=1,\ldots,\nu. \tag{2.7}$$

where $a_i<a_j$ if $i<j$. We write

$$\begin{aligned}F_a={}&{}_1F_aI+{}_3F_{aa_1a_2}\gamma_{a_1}\gamma_{a_2}+\cdots\\&+{}_{2\nu+1}F_{aa_1\cdots a_{2\nu}}\gamma_{a_1}\cdots\gamma_{a_{2\nu}}\\&+{}_2F_{aa_1}\omega\gamma_{a_1}+\cdots+{}_{2\nu}F_{aa_1\cdots a_{2\nu-1}}\omega\gamma_{a_1}\cdots\gamma_{a_{2\nu-1}},\end{aligned} \tag{2.8}$$

where we take ${}_pF_{aa_1\cdots a_{p-1}}={}_pF_{a[a_1\cdots a_{p-1}]}$. The square bracket denotes complete antisymmetrization. The conditions (2.5a) then imply

$${}_pF_{a_0\cdots a_{p-1}}={}_pF_{[a_0\cdots a_{p-1}]}. \tag{2.9}$$

In particular

$${}_{2\nu+1}F_{a_0a_1\cdots a_{2\nu}}=0 \text{ and } {}_{2\nu}F_{a_0a_1\cdots a_{2\nu-1}}=C\epsilon_{0,1,\ldots,2\nu-1}.$$

The conditions (2.5b) then imply

$$\begin{aligned}&[1/p!]P_{a_0'\cdots a_{p-1}'}\left[\partial_{a_0'}\left({}_pF_{aa_1'\cdots a_{p-1}'}\right)\right]\\&\quad+\partial_c\left({}_{p+2}F_{aca_0\cdots a_{p-1}}\right)+2\left({}_{p+2}G_{aa_0\cdots a_{p-1}}\right)=0,\end{aligned} \tag{2.10}$$

where round brackets denote symmetrization, the first summation is over all permutations $a_0'\cdots a_{p-1}'$ of the fixed set $a_0,\cdots,a_{p-1}$, and $P_{a_0'\cdots a_{p-1}'}$ is the sign of this permutation. From these equations we can deduce that

$$\partial_b\left({}_pF_{aa_1\cdots a_{p-1}}\right)+\partial_a\left({}_pF_{ba_1\cdots a_{p-1}}\right)=0, \tag{2.11}$$

i.e., each ${}_pF_{a_1\cdots a_p}$ function is a generalized Killing–Yano tensor.[11] In particular, $\partial_aC=0$ and $\partial_b({}_1F_a)+\partial_a({}_1F_b)=0$. This last condition is just the statement that the ${}_1F_a$ are the components of a Killing vector. The remaining conditions are, in fact, redundant, since, for any general Killing–Yano tensor[11] ${}_pF_{a_1\cdots a_p}$, we have that

$$\partial_a\,\partial_b\left({}_pF_{a_1\cdots a_p}\right)=0. \tag{2.12}$$

We thus see that the space of operators L is determined by the Killing–Yano tensors ${}_pF_{a_1\cdots a_p}$ and ${}_{p+1}G_{a_0\cdots a_{p+1}}$ via (2.10)

The general solution of the Killing–Yano equations (2.11) is known[11] to be

$${}_pF_{a_1\cdots a_p}(z_1,\ldots,z_n)=Az_i\epsilon_{ia_1\cdots a_p}+B\epsilon_{a_1\cdots a_p} \tag{2.13}$$

and the corresponding solutions for

$$\begin{aligned}{}_{p+2}G_{aa_1\cdots a_p}&=\tfrac{1}{2}p\,\partial_a\left({}_pF_{a_1\cdots a_p}\right)\\&=A\,\tfrac{1}{2}p\epsilon_{aa_1\cdots a_p}.\end{aligned} \tag{2.14}$$

A basis for the space $\{L\}$ consists of

$$\begin{aligned}L_{2q}={}&[1/(2q)!]P_{a'b'a_1'\cdots a_{2q}'}z_{a'}\,\partial_{b'}\,\gamma_{a_1'}\cdots\gamma_{a_{2q}'}\\&+q\gamma_a\gamma_b\gamma_{a_1}\cdots\gamma_{a_{2q}},\quad q=0,1,\ldots,\nu,\end{aligned} \tag{2.15}$$

$$\begin{aligned}L_{2q-1}={}&[1/(2q-1)!]P_{a'b'a_1'\cdots a_{2q-1}'}z_{a'}\,\partial_{b'}\,\omega\gamma_{a_1'}\cdots\gamma_{a_{2q-1}'}\\&+(q-\tfrac{1}{2})\omega\gamma_a\gamma_b\gamma_{a_1}\cdots\gamma_{a_{2q-1}},\quad q=1,\ldots,\nu,\end{aligned} \tag{2.16}$$

$$M_{2q}=[1/(2q)!]P_{b'a_1'\cdots a_{2q}'}\,\partial_{b'}\,\gamma_{a_1'}\cdots\gamma_{a_{2q}'},\quad q=0,1,\ldots,\nu, \tag{2.17}$$

$$M_{2q-1}=[1/(2q-1)!]P_{b'a_1'\cdots a_{2q-1}'}\,\partial_{b'}\,\omega\gamma_{a_1'}\cdots\gamma_{a_{2q-1}'}, \tag{2.18}$$

where the summations extend over a fixed set of indices (e.g., a, b, $a_1,\ldots,a_{2q}$ in the case of L_{2q}). This basis has a particular significance, which we can see as follows: consider operators of the type M_l. From (2.17) and (2.18) we have

$$M_l^2=\partial_b^2+\cdots+\partial_l^2, \tag{2.19}$$

i.e., M_l^2 is the second-order Casimir invariant for the subgroup E_{l+1}, whose Lie algebra has the basis

$$\begin{aligned}&P_\lambda=\partial_\lambda,\\&M_{\lambda\mu}=z_\lambda\,\partial_\mu-z_\mu\,\partial_\lambda+\tfrac{1}{2}\gamma_\lambda\gamma_\mu,\\&\lambda,\mu=b,a_1,\ldots,a_l,\quad\lambda\neq\mu.\end{aligned} \tag{2.20}$$

A similar result holds for the operators L_l; from (2.15) and (2.16) it follows that

$$L_l^2=\sum_{\lambda>\mu}M_{\lambda\mu}^2+\frac{1}{8}l(l+1)I_n, \tag{2.21}$$

i.e., to within a constant L_l^2 is the Casimir invariant for the subgroup $SO(l+1)$, whose Lie algebra has a basis

$$M_{\lambda\mu},\quad\lambda,\mu=1,b,a_1,\ldots,a_l,\quad\lambda>\mu.$$

These operators generalize the "square root of angular momentum" introduced by Dirac in this treatment of the electron.

It is in fact the study of orbits of commuting operators that should be of basic importance to a study of separation of variables. The particular example of Chandrasekhar[5] has highlighted this feature. From the point of view of separation of variables theory the operators that are associated with it could be second order. As a step in this direction we extend the studies of McLenaghan to second-order matrix differential operators that commute with H.

III. SECOND-ORDER CONSTANTS OF THE MOTION FOR THE DIRAC HAMILTONIAN IN E_4

In this section we study second-order operators of the type

$$\hat{\mathscr{L}}=K_{ab}\,\partial_a\,\partial_b+L_c\,\partial_c+M, \tag{3.1}$$

which commute with the Dirac Hamiltonian in complex Euclidean four-space. (To make the computations relatively straightforward we restrict ourselves to E_4.) The condition $[H,\hat{\mathscr{L}}]=0$ is equivalent to the equations

$$[\gamma_{(a},K_{bc)}]=0, \tag{3.2a}$$

$$-2\gamma_d(\partial_dK_{ab})+[\gamma_{(a},L_{b)}]=0, \tag{3.2b}$$

$$\gamma_d(\partial_d L_a) + [\gamma_a, M] = 0, \tag{3.2c}$$

$$\gamma_d(\partial_d M) = 0, \tag{3.2d}$$

where the ( ) subscripts denote complete symmetrization of the enclosed indices.

Our purpose is to show that all second-order constants of the motion of the type (2.1) can be constructed as products of the first-order ones, as calculated in Sec. II. We note that the set $\{\hat{\mathscr{L}}\}$ does not close under commutation; however, if L_1, L_2 are any two first-order matrix differential operators that commute with H, then $[L_1 L_2, H] = 0$.

A suitable basis for $\{L\}$ in E_4 is

$$L_{abc} = \gamma_5[\gamma_{(a} z_b \partial_{c)} - \gamma_{(a} z_c \partial_{b)}] + \gamma_d, \quad a>b>c, \quad a,b,c,d \neq, \tag{3.3a}$$

$$Q_{ab} = \gamma_5 \gamma_{[a} \partial_{b]}, \quad a>b, \tag{3.3b}$$

$$S_{abc} = \gamma_{(a}\gamma_b \partial_{c)}, \quad a>b>c, \tag{3.3c}$$

$$M = \epsilon_{abcd}\gamma^a\gamma^b z_c \partial_d + \tfrac{3}{2}\gamma_5, \tag{3.3d}$$

$$M_{ab} = z_{[a} \partial_{b]} + \tfrac{1}{2}\gamma_a\gamma_b, \quad a>b, \tag{3.3e}$$

$$P_i = \partial_i, \tag{3.3f}$$

$$H = \gamma_i \partial_i \tag{3.3g}$$

where all indices run from 1,...,4. From the first of conditions (3.2), if we write

$$K_{ab} = K_{ab} I + K_{abc}\gamma_c + K_{abcd}\gamma_c\gamma_d + \hat{K}_{abc}\gamma_5\gamma_c + \hat{K}_{ab}\gamma_5, \tag{3.4}$$

then the coefficients of K_{ab} must satisfy

$$K_{(abc)d} = 0, \tag{3.5}$$

$$K_{bcd}(\delta_{a\alpha}\delta_{d\beta} - \delta_{a\beta}\delta_{d\alpha}) + K_{acd}(\delta_{b\alpha}\delta_{d\beta} - \delta_{b\beta}\delta_{d\alpha}) + K_{abd}(\delta_{c\alpha}\delta_{d\beta} - \delta_{c\beta}\delta_{d\alpha}) = 0, \tag{3.6}$$

$$\hat{K}_{(abc)} = 0, \tag{3.7}$$

$$\hat{K}_{ab} = 0, \tag{3.8}$$

in addition to the obvious symmetries

$$K_{[ab]} = 0, \tag{3.9}$$

$$K_{ab(cd)} = 0. \tag{3.10}$$

For the second set of conditions (3.2) we write

$$L_a = L_a I + L_{ab}\gamma_b + L_{abc}\gamma_b\gamma_c + \hat{L}_{ab}\gamma_5\gamma_b + \hat{L}_a\gamma_5, \tag{3.11}$$

with $L_{a(bc)} = 0$ and obtain

$$\partial_c K_{ab} + L_{(ab)c} + \partial_d K_{abdc} = 0, \tag{3.12}$$

$$\partial_{(c}K_{|ab|de)} + \epsilon_{fcde}\partial_f \hat{K}_{ab} + 2L_b\epsilon_{acde} + 2L_a\epsilon_{bcde} = 0, \tag{3.13}$$

$$\epsilon_{cdfe}\partial_c(K_{abd}) + \partial_{[f}\hat{K}_{|ab|e]} + \epsilon_{acfe}L_{bc} + \epsilon_{bcfe}L_{ac} = 0, \tag{3.14}$$

$$\partial_d(\hat{K}_{abd}) + 2(\hat{L}_{ab} + \hat{L}_{ba}) = 0, \tag{3.15}$$

$$\partial_c K_{abc} = 0. \tag{3.16}$$

For the third set of conditions, we write

$$M = MI + M_a\gamma_a + M_{ab}\gamma_a\gamma_b + M_c\gamma_5\gamma_c + M\gamma_5 \tag{3.17}$$

and obtain the conditions

$$\partial_c L_{ac} = 0, \tag{3.18}$$

$$\partial_b L_a + \partial_c L_{abc} - 2M_{ab} = 0, \tag{3.19}$$

$$\partial_{(b}L_{|a|cd)} + \epsilon_{ebcd}\partial_e\hat{L}_a + 2\epsilon_{abcd}\hat{M} = 0, \tag{3.20}$$

$$\partial_{[b}\hat{L}_{|a|c]} + \epsilon_{decb}\partial_d L_{ae} + 2\epsilon_{adcb}M_d + 2\epsilon_{bdcb}M_d = 0, \tag{3.21}$$

$$\partial_c\hat{L}_{ac} + 2\hat{M}_a = 0. \tag{3.22}$$

We will now show that the space of operators L in E_4 is spanned by all products of first-order matrix operators. From (3.12) and (3.5) we can see that

$$\partial_{(c}K_{ab)} = 0. \tag{3.23}$$

There are 50 independent operators $\tilde{L}$ of the form

$$\tilde{L} = K_{ab}\partial_a\partial_b + L_{abc}\gamma_b\gamma_c\partial_a + M \tag{3.24}$$

constructed from the symmetric products in the enveloping algebra, i.e., products of the form $\{P_i,P_j\}$, $\{P_i,M_{jk}\}$, $\{M_{ij},M_{kl}\}$. The conditions (3.23) are the equations for a symmetric Killing tensor to exist in four-dimensional flat space E_4. These conditions have been discussed by Katzin and Levin[14] and the above result is included in their work.

From (2.6) we deduce that

$$K_{abc} = 0, \quad a,b,c\neq, \tag{3.25}$$

$$-K_{aaa} + 2K_{abb} = 0, \quad a\neq b, \tag{3.26}$$

and consequently

$$K_{abc} = K_a\delta_{ac}. \tag{3.27}$$

From (2.16) we have that

$$\partial_a K_b + \partial_b K_a = 0;$$

these are just Killing's equations. There are therefore ten independent operators of the form

$$\hat{L} = K_{abc}\gamma_c\partial_a\partial_b + \hat{L}_{ab}\gamma_5\gamma_b\partial_a + L_{ab}\gamma_b\partial_a. \tag{3.28}$$

These operators are formed by taking symmetric products of the form $\{H, P_i\}$, $\{H,M_{ij}\}$.

From (3.7) and (3.14) we deduce that

$$\hat{K}_{(abc)} = 0, \tag{3.7}$$

$$\partial_{(a}\hat{K}_{bc)d} = 0. \tag{3.29}$$

The number of independent solutions can be calculated as follows. We note that for fixed d, $K^{(d)}_{bc} = \hat{K}_{bcd}$ satisfies the equations for a second-order Killing tensor in four-dimensional Euclidean space, i.e.,

$$\partial_{(a}K^{(d)}_{bc)} = 0. \tag{3.30}$$

It is known[14] that the vector space of second-order Killing tensors is in this case of dimension 50. Furthermore it is always possible to choose a basis of the form

$$\kappa^l_{bc} = A^{\ l}_{bc,ef} z_e z_f, \quad l = 1,...,20,$$

$$\mu^m_{bc} = B^{\ m}_{bc,e} z_e, \quad m = 1,...,20,$$

$$\nu^n_{bc} = C^{\ n}_{bc}, \quad n = 1,...,10, \tag{3.31}$$

where $A^{\ l}_{bc,ef}$, $B^{\ l}_{bc,e}$, and $C^{\ l}_{bc}$ are constants. Consequently because of (3.30) we may write

$$K^{(d)}_{bc} = c^{dl}\kappa^l_{bc} + d^{\ dm}\mu^m_{bc} + e^{dn}\nu^n_{bc}. \tag{3.32}$$

Our problem is to determine the number of independent coefficients c^{dl}, $d^{\ dm}$, e^{dn}, given that the $\hat{K}_{abc}$ are subject to the conditions (3.7) and

$$\partial_d\hat{K}_{(abc)} = 0, \tag{3.7}$$

$$\partial_d \partial_e \hat{K}_{(abc)} = 0. \tag{3.33}$$

To determine the number of independent coefficients e^{dn} consider the $\hat{K}_{abc}$ evaluated at **0**, i.e., $\hat{K}_{abc}(\mathbf{0})$. There are 40 such coefficients and they are subjected to 20 independent constraints $\hat{K}_{(abc)}(\mathbf{0}) = 0$. There are therefore 20 independent constants e^{dn}. These are constructed from the 24 anticommutators $\{P_c, Q_{ab}\}$ subject to the four constraints

$$Q_{(ab}P_{c)} = 0. \tag{3.34}$$

To determine the number of independent coefficients d^{dm} we consider $\partial_a \hat{K}_{bcd}(\mathbf{0})$. There are 80 unknown coefficients d^{dm} subject to the 51 constraints

$$\begin{aligned}
&\partial_a \hat{K}_{daa}(\mathbf{0}) = 0, \quad a \neq d,\\
&\partial_d \hat{K}_{aad}(\mathbf{0}) + 2\partial_d \hat{K}_{add}(\mathbf{0}) = 0, \quad a \neq d,\\
&\partial_c \hat{K}_{(aab)}(\mathbf{0}) = 0, \quad a,b,c \neq,\\
&\partial_a \hat{K}_{(abc)}(\mathbf{0}) = 0, \quad a,b,c \neq,\\
&\partial_d \hat{K}_{(abc)}(\mathbf{0}) = 0, \quad a,b,c,d \neq.
\end{aligned} \tag{3.35}$$

All indices are distinct in these conditions and conditions of the last type are subject to the restriction

$$\partial_a \hat{K}_{(bcd)}(\mathbf{0}) + \partial_b \hat{K}_{(cda)}(\mathbf{0}) + \partial_c K_{(dab)}(\mathbf{0}) + \partial_d \hat{K}_{(abc)}(\mathbf{0}) = 0,$$

which follows from conditions (3.29).

A suitable basis for operators associated with these independent constants is obtained from the 52 anticommutators $\{P_a, L_{bcd}\}$, $\{M_{ab}, Q_{cd}\}$ subject to the 23 independent constraints

$$\begin{aligned}
&Q_{(ab}M_{c)d} = L_{abc}P_d + H/2,\\
&Q_{[a|b}M_{b|c]} = Q_{ca} - L_{abc}P_b,\\
&P_{[a}L_{bc|d]} = -M_{bc}Q_{ad} + M_{ad}Q_{bc},\\
&\sum_{\substack{a>b\\c>d}} \epsilon_{abcd}M_{ab}Q_{cd} + \frac{H}{2} = 0.
\end{aligned} \tag{3.36}$$

To determine the number of independent coefficients c^{dl} we consider the second derivatives $\partial_a \partial_b \hat{K}_{cde}(\mathbf{0})$. There are 80 unknown coefficients c^{dl} subject to 60 constraints:

$$\begin{aligned}
&\partial_a \hat{K}_{daa}(\mathbf{0}) = 0, \quad \partial_d \partial_a \hat{K}_{daa}(\mathbf{0}) = 0, \quad a \neq d,\\
&\partial_c \partial_a \hat{K}_{daa}(\mathbf{0}) = 0, \quad a,c,d \neq,\\
&\partial_c^2(\hat{K}_{aab}(\mathbf{0}) + 2\hat{K}_{baa}(\mathbf{0})) = 0, \quad ab,c \neq,\\
&\partial_c \partial_d(\hat{K}_{aab}(\mathbf{0}) + 2\hat{K}_{baa}(\mathbf{0})) = 0, \quad a,b,c \neq.
\end{aligned} \tag{3.37}$$

A suitable basis for operators associated with these independent constants is obtained from the 24 anticommutators $\{M_{ab}, L_{cde}\}$ subject to the four constraints

$$M_{a(b}L_{|a|cd)} = L_{bcd}. \tag{3.38}$$

From (3.5) and (3.13) we have the conditions

$$K_{(abc)d} = 0, \tag{3.39}$$

$$\partial_{(a}K_{bc)de} = 0. \tag{3.40}$$

We are, of course, also assuming that $K_{abcd} = K_{(ab)cd}$ and $K_{abcd} = K_{ab[cd]}$. Conditions (3.39) are then equivalent to the four types

$$K_{abcd} + K_{cabd} + K_{bcad} = 0, \quad a,b,c,d \neq, \tag{3.41a}$$

$$K_{acca} = 0, \quad a, \neq c, \tag{3.41b}$$

$$K_{aacd} + 2K_{caad} = 0, \quad a,c,d \neq, \tag{3.41c}$$

$$K_{aaad} = 0, \quad a, \neq d. \tag{3.41d}$$

Conditions (3.40) are equivalent to the five types

$$\partial_a K_{bcce} + \partial_c K_{abce} + \partial_b K_{acce} = 0, \quad a,b,c,e \neq, \tag{3.42a}$$

$$\partial_a K_{bccb} + \partial_c K_{bacb} + \partial_b K_{accb} = 0, \quad a,b,c \neq, \tag{3.42b}$$

$$2\partial_a K_{acde} + \partial_c K_{aade} = 0, \quad a,c,d,e \neq, \tag{3.42c}$$

$$2\partial_a K_{acce} + \partial_c K_{aace} = 0, \quad a,c,e \neq, \tag{3.42d}$$

$$\partial_a K_{aade} = 0, \quad a,d,e \neq. \tag{3.42e}$$

The number of independent solutions of these equations again can be determined by the constants $K_{abcd}(\mathbf{0})$ and all possible derivatives of K_{abcd} evaluated at **0**. The number of independent components of $K_{abcd}(\mathbf{0})$ is 60 and the number of constraints of type (3.29) is 34. The number of derivatives $\partial_e K_{abcd}(\mathbf{0})$ is 240. The number of constraints on the first derivatives are obtained by counting the number of independent constraints from (3.40) and the derivatives of (3.39). There are 136 such conditions, as it can readily be verified that all the conditions so obtained are independent. If we now repeat these considerations for the derivatives $\partial_e \partial_f K_{abcd}(\mathbf{0})$ we obtain at first glance 600 such derivatives and 628 conditions on them obtained by differentiating conditions (3.39) twice and conditions (3.40) once. There are, in fact, only 600 independent conditions. This can be seen as follows. From the conditions

$$\begin{aligned}
&\partial_a(2\partial_a K_{acde} + \partial_c K_{aade}) = 0, \quad a,c,d,e \neq,\\
&\partial_e \partial_a K_{aade} = 0, \quad e,a,d \neq,
\end{aligned} \tag{3.43}$$

we deduce that

$$\partial_a^2 K_{acde} = 0, \quad a,c,d,e \neq. \tag{3.44}$$

Differentiating (3.41c) with respect to ∂_a and using (3.42e) we have that $\partial_a K_{caad} = 0$. Consequently the four conditions

$$\partial_c(\partial_a K_{bcce} + \partial_c K_{abce} + \partial_b K_{acce}) = 0, \quad a,b,c,e \neq, \tag{3.45}$$

which are obtained from (3.42a), are redundant.

Further, the conditions

$$\partial_a(2\partial_a K_{acce} + \partial_c K_{aace}) = 0, \quad a \neq c, \tag{3.46}$$

$$\partial_c \partial_a K_{aadc} = 0, \quad c,a,d \neq, \tag{3.47}$$

imply that

$$\partial_a^2 K_{acce} = 0, \quad a,c,e \neq. \tag{3.48}$$

The condition

$$\partial_c^2(K_{aacd} + 2K_{caad}) = 0, \quad a,c,d \neq, \tag{3.49}$$

then implies

$$\partial_c^2 K_{aacd} = 0, \quad a,c,d \neq. \tag{3.50}$$

Then condition

$$\partial_b(\partial_c K_{bacd} + \partial_b K_{accb}) = 0, \quad a,b,c \neq, \tag{3.51}$$

implies that

$$\partial_b \partial_c K_{abbc} = 0, \quad a,b,c \neq. \tag{3.52}$$

Now conditions

$$\partial_a \partial_d (K_{aacd} + 2K_{caad}) = 0, \quad c,a,d \neq, \tag{3.53}$$

also imply (3.52), so they are redundant. There are 24 of them. Thus we have succeeded in showing that there are only 600 independent conditions on the second derivatives $\partial_e \partial_f K_{abcd}(0)$. In fact, apart from the redundancies noted above, all these conditions are independent. These computations indicate that there must be 58 independent solutions to our original conditions. These solutions can be generated by anticommutators $\{H,Q_{ab}\}$, $\{H,L_{abc}\}$, $\{M,M_a\}$, $\{M,P_i\}$, $\{S_{abc},M_{ij}\}$, $\{S_{abc},P_i\}$. There are 60 of these combinations but there are two independent relations among them:

$$S_{(abc}P_{d)} = 0, \tag{3.54}$$

$$\sum_{i>j>k} L_{ijk}(P_i + P_j + P_k) + \left(\sum_{i>j} Q_{ij}\right)H = 0. \tag{3.55}$$

Theorem 1: Let $H = \gamma_a \partial_a + m$ be the Dirac operator in complex Euclidean four-space. Further let $\mathscr{L} = \{L\}$ be the space of all first-order differential operators $L = F_a \partial_a + G$ that commute with H. Then the space $\hat{\mathscr{L}} = \{\hat{L}\}$, consisting of all second-order operators of the type $\hat{L} = K_{ab} \partial_a \partial_b + L_c \partial_c + M, K_{ab} \not\equiv 0$, that commute with H, is spanned by all products of element pairs of elements of $\mathscr{L}$.

Theorem 1 suggests that higher-order operators that commute with the Dirac operator also can be constructed as products of first-order symmetries, but we have not proved this.

IV. SEPARATION OF VARIABLES FOR THE DIRAC EQUATION IN MINKOWSKI SPACE

In this section we discuss how the first-order matrix operators L that commute with the Dirac Hamiltonian can be associated with separable solutions of Dirac's equation. This was implicitly shown by Chandrasekhar's analysis[5] of Dirac's equation in a Kerr background and explicitly by the detailed study[8] of Carter and McLenaghan. In the limiting case, where the Kerr metric degenerates to a flat space metric in oblate spheroidal coordinates, we have infinitesimal distance

$$ds^2 = dt^2 - \left[\frac{r^2 + a^2\cos^2\theta}{(r^2 + a^2)}dr^2 + (r^2 + a^2\cos^2\theta)d\theta^2 + (r^2 + a^2)\sin^2\theta\, d\phi^2\right]. \tag{4.1}$$

A more familiar version of this infinitesimal distance can be obtained by putting $r = a \sinh \eta$:

$$ds^2 = dt^2 - a^2[(\sinh^2\eta + \cos^2\theta)(d\eta^2 + d\theta^2) + \cosh^2\eta \sin^2\theta\, d\phi^2]. \tag{4.2}$$

Dirac's equation in Newman–Penrose notation is

$$(D + \epsilon - p)F_1 + (\delta^* + \pi - \alpha)F_2 = imG_1,$$
$$(\Delta + \mu - \gamma)F_2 + (\delta + \beta - \tau)F_1 = imG_2,$$
$$(D + \epsilon^* - p^*)G_2 - (\delta + \pi^* - \alpha^*)G_1 = imF_2,$$
$$(\Delta + \mu^* - \gamma^*)G_1 - (\delta + \beta^* - \tau)G_2 = imF_1.$$

Here we have used Chandrasekhar's[5] notation for the spin coefficients and derivatives. A distinguishing feature of spinor equations is that the specification of coordinates does not determine uniquely the resulting form of the equation; one also needs to specify a (null) tetrad or moving reference frame in order to write the resulting equation. These ideas have their natural framework in the tetrad formalism.[5]

The first-order operators L, which commute with the Dirac operator H, are of crucial importance for the separable solutions of Dirac's equation computed by Chandrasekhar. We briefly review his procedure. Essentially Chandrasekhar has shown that Dirac's equation in a Kerr space-time background admits a solution which can be obtained from a separation of variables ansatz. Since oblate spheroidal coordinates in Minkowski space are a special case of the standard Kerr space-time metric, this implies that the Dirac equation in Minkowski space admits separable solutions in these coordinates.

What is interesting about Chandrasekhar's result is that the proper choice of null tetrad is unexpected. If we adopt coordinates t, r, θ, and ϕ, corresponding to the infinitesimal distance (4.1), the proper null tetrad has the components

$$l^i = (1,1,0,a/(r^2 + a^2)), \tag{4.3a}$$
$$n^i = [1/2(r^2 + a^2\cos^2\theta)](r^2 + a^2, -r^2 - a^2, 0, a), \tag{4.3b}$$
$$m^i = [1/\sqrt{2}(r + ia\cos\theta)](ia\sin\theta, 0, 1, i/\sin\theta). \tag{4.3c}$$

This is quite different from the appropriate choice in, say, the case of cylindrical coordinates with infinitesimal distance

$$ds^2 = dt^2 - dr^2 - r^2\, d\phi^2 - dz^2, \tag{4.4}$$
$$l^i = (1/\sqrt{2})(1,0,0,1), \tag{4.5a}$$
$$n^i = (1/\sqrt{2})(1,0,0,-1), \tag{4.5b}$$
$$m^i = (1/\sqrt{2})(0,1,i/r,0). \tag{4.5c}$$

This frame is simply related to the frame of orthogonal vectors

$$e^i_t = (1/\sqrt{2})(l^i + n^i), \quad e^i_z = (1/\sqrt{2})(l^i - n^i),$$
$$e^i_r = (1/\sqrt{2})(m^i + \bar{m}^i), \quad e^i_\phi = (1/\sqrt{2})(m^i - \bar{m}^i), \tag{4.6}$$

where

$$e^i_\lambda e_{\mu i} = 0, \quad \text{if } \lambda \neq \mu,$$
$$e^i_\lambda e_{\lambda i} = \epsilon_\lambda,$$

$\epsilon_\lambda = +1$ if $\lambda = 1$ and -1 otherwise. For all coordinate systems that are characterized by the Casimir operators of some subgroup chain of the Poincaré group E(3,1), a choice of tetrad of this type will yield separable solutions and uncoupled equations.[15] There are sound group theoretical reasons for this, which we do not elaborate on here. Now the obvious choice for oblate spheroidal coordinates would be a null tetrad constructed via (4.6) from the orthogonal vectors

$$\tilde{e}^a_t = (1,0,0,0),$$
$$\tilde{e}^a_r = -\sqrt{(r^2 + a^2)/(r^2 + a^2\cos^2\theta)}\,(0,1,0,0),$$
$$\tilde{e}^a_\theta = (1/\sqrt{r^2 + a^2\cos^2\theta})(0,0,1,0), \tag{4.7}$$
$$\tilde{e}^a_\phi = (1/\sin\theta\sqrt{r^2 + a^2})(0,0,0,1).$$

However, this choice does not lead to separable solutions. With the proper null tetrad (4.3) and

$$f_1 = (r - ia\cos\theta)F_1, \quad f_2 = F_2,$$
$$g_2 = (r + ia\cos\theta)G_2, \quad g_1 = G_1, \tag{4.8}$$

Dirac's equation becomes

$$\begin{aligned}
&\mathscr{D}_0 f_1 + 2^{-1/2}\mathscr{L}_{1/2} f_2 = m(ir + a\cos\theta)g_1,\\
&\Delta\mathscr{D}^{\dagger}_{1/2} f_2 - 2^{1/2}\mathscr{L}_{1/2} f_1 = -2m(ir + a\cos\theta)g_2,\\
&\mathscr{D}_0 g_2 - 2^{-1/2}\mathscr{L}^{\dagger}_{1/2} g_1 = m(ir - a\cos\theta) f_2,\\
&\Delta\mathscr{D}^{\dagger}_{1/2} g_1 + 2^{1/2}\mathscr{L}_{1/2} g_2 = -2m(ir - a\cos\theta) f_1,
\end{aligned} \tag{4.9}$$

where

$$\mathscr{D}_0 = \partial_r + iK/\Delta, \quad \mathscr{D}^{\dagger}_{1/2} = \partial_r - iK/\Delta + r/\Delta,$$
$$\mathscr{L}_{1/2} = \partial_\theta + Q + \tfrac{1}{2}\cot\theta, \quad \mathscr{L}^{\dagger}_{1/2} = \partial_\theta - Q + \tfrac{1}{2}\cot\theta,$$

and

$$K = (r^2 + a^2)\sigma + am^*, \quad Q = a\sigma\sin\theta + m^*\csc\theta.$$

In these equations the t and ϕ dependence has been removed by assuming it to be of the form $e^{i(\sigma t + m^*\phi)}$ and factored out. These equations admit a separable solution if we make the substitution

$$f_1 = R_{-1/2}(r)S_{-1/2}(\theta), \quad f_2 = R_{1/2}(r)S_{1/2}(\theta),$$
$$g_1 = R_{1/2}(r)S_{-1/2}(\theta), \quad g_2 = R_{-1/2}(r)S_{1/2}(\theta). \tag{4.10}$$

The functions appearing in this substitution can be chosen to satisfy

$$\begin{aligned}
&\Delta^{1/2}\mathscr{D}_0 R_{-1/2} = (\lambda + imr)\Delta^{1/2}R_{1/2},\\
&\Delta^{1/2}\mathscr{D}^{\dagger}_0\Delta^{1/2}R_{1/2} = (\lambda - imr)R_{-1/2},\\
&\mathscr{L}_{1/2}S_{1/2} = -(\lambda - am\cos\theta)S_{-1/2},\\
&\mathscr{L}^{\dagger}_{1/2}S_{-1/2} = (\lambda + am\cos\theta)S_{1/2},
\end{aligned} \tag{4.11}$$

where λ is a separation constant. If we write ψ as the column vector (f_1, f_2, g_1, g_2) the Dirac's equation has the form $H\psi = m\psi$.

The separation constant is also the eigenvalue of an operator L; i.e.,

$$L\psi = \lambda\psi, \tag{4.12}$$

where

$$L = \begin{bmatrix}
0 & 0 & (ia\cos\theta/2\rho)\Delta\mathscr{D}^{\dagger}_{1/2} & (-r/\sqrt{2}\rho)\mathscr{L}_{1/2}\\
0 & 0 & (r/\sqrt{2}\rho)\mathscr{L}^{\dagger}_{1/2} & (ia\cos\theta/\rho)\mathscr{D}_0\\
(-ia\cos\theta/\rho^*)\mathscr{D}_0 & (r/\sqrt{2}\rho^*)\mathscr{L}_{1/2} & 0 & 0\\
(r/\sqrt{2}\rho^*)\mathscr{L}^{\dagger}_{1/2} & (-ia\cos\theta/2\rho^*)\Delta\mathscr{D}^{\dagger}_{1/2} & 0 & 0
\end{bmatrix}. \tag{4.13}$$

In addition we have that $[H,L] = 0$, so L is a first-order matrix symmetry operator. In fact,[8]

$$L = (1/\sqrt{2})(\tilde{L}_{234} + a\tilde{Q}_{14}), \tag{4.14}$$

where the operators $\tilde{L}$ are those obtained from (3.3) for the corresponding realization in Minkowski space. In this particular case

$$\begin{aligned}
\tilde{L}_{234} &= \gamma^5\gamma^2(x^4\partial_3 - x^3\partial_4) + \gamma^5\gamma^3(x^2\partial_4 - x^4\partial_2)\\
&\quad + \gamma^5\gamma^4(x^3\partial_2 - x^2\partial_3) + \gamma^1,\\
\tilde{Q}_{14} &= \gamma^5\gamma^1\partial_4 + \gamma^5\gamma^4\partial_1,
\end{aligned} \tag{4.15}$$

where the γ^i matrices satisfy

$$\{\gamma^i,\gamma^j\} = g^{ij},$$

where $g^{ij} = \mathrm{diag}(1,-1,-1,-1)$ and contravariant coordinates x^i, $i = 1,2,3,4$.

If one is to construct a satisfactory theory of variable separation for equations of Dirac type, examples of this type need to be explained. In fact, from our knowledge of separable systems for the scalar wave equation we can construct additional such examples of separation. Consider, for instance, the coordinates

$$\begin{aligned}
&t = r\cosh\theta, \quad x = \sqrt{r^2 + a^2}\sinh\theta\cos\phi\\
&y = \sqrt{r^2 + a^2}\sinh\theta\sin\phi, \quad z = z,\\
&0 \leqslant r < \infty, \quad -\infty < \theta < \infty, \quad 0 \leqslant \theta < 2\pi, \quad -\infty < z < \infty.
\end{aligned} \tag{4.16}$$

This is clearly a slightly different variation of oblate spheroidal coordinates. The appropriate null tetrad has contravariant components

$$\begin{aligned}
&l^i = (1,0,a/(r^2 + a^2),1),\\
&n^i = [1/2(r^2 + a^2\cosh^2\theta)](r^2 + a^2,0,-a,-r^2 - a^2),\\
&m^i = [1/\sqrt{2}(r + ia\cosh\theta)](0,1,i/\sinh\theta,ia\sinh\theta).
\end{aligned} \tag{4.17}$$

These coordinates (4.16) and (4.17) enable Dirac's equation to be written as

$$\left(D_+ + \frac{1}{\bar{\eta}^*}\right)F_1 + \frac{1}{\sqrt{2}\bar{\eta}^*}\left(\mathscr{L}_- + \frac{1}{2}\coth\theta\right)F_2 = imG_1, \tag{4.18a}$$

$$\frac{(r^2 + a^2)}{2(r^2 + a^2\cosh^2\theta)}\left(D_- + \frac{2}{(r^2 + a^2)}\right)F_2 + \frac{1}{\sqrt{2}\bar{\eta}}\left(\mathscr{L}_+ + \frac{1}{2}\coth\theta - \frac{ia\sinh\theta}{\bar{\eta}^*}\right)F_1 = imG_2, \tag{4.18b}$$

$$\left(D_+ + \frac{1}{\bar{\eta}}\right)G_2 - \frac{1}{\sqrt{2}\bar{\eta}}\left(\mathscr{L}_- + \frac{1}{2}\coth\theta\right)G_1 = imF_2, \tag{4.18c}$$

$$\frac{(r^2 + a^2)}{2(r^2 + a^2\cosh^2\theta)}\left(D_- + \frac{r}{(r^2 + a^2)}\right)G_1 - \frac{1}{\sqrt{2}\bar{\eta}^*}\left(\mathscr{L}_- + \frac{1}{2}\coth\theta + \frac{ia\sinh\theta}{\bar{\eta}}\right)G_2 = imF_1, \tag{4.18d}$$

where $D_{\pm} = \partial_r \pm iam^*/(r^2+a^2) \pm i\tau$,

$$\mathscr{L}_{\pm} = \partial_\theta \mp (m^*/\sinh\theta) \pm a\tau\sinh\theta, \quad \bar{\eta} = r + ia\cosh\theta,$$

and we have assumed ϕ, z dependence to be $e^{i(m^*\phi+\tau z)}$.

Putting $f_1 = \bar{\eta}^* F_1$, $g_2 = \bar{\eta} G_2$, $f_2 = F_2$, and $g_1 = G_1$, we can verify that separation of variables can be achieved via the substitution (4.10) and the coupled first-order equations

$$D_+ R_{-1/2} = (\lambda + mr) R_{1/2} \tag{4.19a}$$

$$D_- R_{-1/2} = (-\lambda + mr) R_{-1/2} \tag{4.19b}$$

$$(-1/2)\mathscr{L}_+ S_{-1/2} = (-\lambda + ima\cosh\theta) S_{+1/2}, \tag{4.19c}$$

$$(-1/2)\mathscr{L}_- S_{1/2} = (\lambda + ima\cosh\theta) S_{-1/2}. \tag{4.19d}$$

The operator whose eigenvalue is the separation parameter is $\tilde{L}_{123} + a\tilde{Q}_{14}$. For a genuinely new separable system differing from spheroidal coordinates consider the infinitesimal distance associated with the coordinate system (4.16),

$$ds^2 = (r^2 + a^2\cosh^2\theta)\left[\frac{dr^2}{(r^2+a^2)} - d\theta^2\right] - (r^2+a^2)\sinh^2\theta\, d\phi^2 - dz^2. \tag{4.20}$$

If we allow r and θ to be large and replace $a/2$ by b and ϕ by $2v$, we obtain the related infinitesimal distance

$$ds^2 = (r^2 + b^2 e^{2\theta})[dr^2/r^2 - d\theta^2] - r^2 e^{2\theta} dv^2 - dz^2. \tag{4.21}$$

We can then associate with this distance the null tetrad

$$l^i = (1,0,b/r^2,1), \tag{4.22a}$$

$$n^i = [r^2/2(r^2+b^2e^{2\theta})](1,0,-b/r^2,-1), \tag{4.22b}$$

$$m^i = [1/\sqrt{2}(r+ibe^{\theta})](0,1,-ie^{-\theta},ibe^{\theta}). \tag{4.22c}$$

This coordinate system and frame clearly afford a separation of variables via the foregoing techniques. The separation equations can be obtained by the appropriate limits from the equations for the previous coordinate system. A suitable choice of space time coordinates is

$$t + x = \frac{1}{b} re^{\theta} v^2 + \frac{r}{b} e^{-\theta} - \frac{b}{r} e^{\theta},$$

$$t - x = bre^{\theta}, \quad y = re^{\theta} v, \quad z = z. \tag{4.23}$$

The operator which describes the separation of the variables r and θ is

$$\tilde{L}_{123} + b(\tilde{Q}_{24} + \tilde{Q}_{14}). \tag{4.24}$$

The examples of coordinate systems given here are based on the mechanism given in Chandrasekhar's original work. Clearly separation of variables for Dirac's equation depends on a simultaneous choice of coordinates and null tetrad. What is the connection between the null tetrad (4.3) and oblate spheroidal coordinates (4.1)? The operator L (4.14) has associated it with a Killing–Yano tensor $D^c{}_b$ with matrix elements

$$D^c{}_b = \begin{bmatrix} 0 & 0 & 0 & a \\ 0 & 0 & -x^4 & x^3 \\ 0 & x^4 & 0 & -x^2 \\ a & -x^3 & x^2 & 0 \end{bmatrix}. \tag{4.25}$$

If we compute the roots and eigenvectors of $D^a{}_b$,

$$(D^c{}_b - \lambda\delta^c{}_b)v^b = 0, \tag{4.26}$$

we obtain

$$(i)\ \lambda = \pm ir, \quad v \sim (\pm ia\sin\theta, 0, 1, \pm i/\sin\theta),$$
$$(ii)\ \lambda = \pm a\cos\theta, \quad v \sim (1, \pm 1, 0, a/(r^2+a^2)). \tag{4.27}$$

Here we have written the eigenvectors relative to the t, r, θ, ϕ moving frame and have chosen Minkowski space-time coordinates as in (4.16). From (4.3) we see that these eigenvectors are, apart from normalization conventions, the basis vectors that define the null tetrad (4.3). We can go further than this. Consider the square of the matrix $D = (D^a{}_b)$. We know[11] that $\mathscr{D}^a{}_b = D^a{}_c D^c{}_b$ is a Killing tensor and, from what we have just observed, the above eigenvectors are also eigenvectors of $D^a{}_b$. In fact the Killing tensor $\mathscr{D}^{ab}$ is intimately related to the choice of coordinates t, r, θ, and ϕ. If we pass to the cotangent bundle (i.e., phase space in Minkowski space-time), then

$$\mathbb{D} = \mathscr{D}^{cb} p_c p_b = m_{23}^2 + m_{24}^2 + m_{34}^2 + ap_1 m_{23} + a^2(p_1^2 - p_4^2), \tag{4.28}$$

where we have used the notation

$$m_{ij} = x^i p x^j - x^j p x^i, \quad i,j = 2,3,4, \tag{4.29}$$

$$p_i = p x^i, \quad i = 1,\ldots,4. \tag{4.30}$$

These linear forms on the cotangent bundle, together with

$$n_{1j} = x^1 p x^j + x^j p x^1, \quad j = 2,3,4, \tag{4.31}$$

form the usual representation of the Poincaré algebra $\epsilon(3,1)$ with the Poisson bracket as commutator.

For additive separation of variables for the Hamilton–Jacobi equation

$$H = g^{cb} p_y c p_y b = p_{x^1}^2 - p_{x^2}^2 - p_{x^3}^2 - p_{x^4}^2 = E, \tag{4.32}$$

expressed in a given coordinate system $\{y^i\}$ (e.g., t, r, θ, ϕ, oblate spheroidal coordinates), there is a complete theory.[16,17]

Theorem: Necessary and sufficient conditions for the existence of an orthogonal separable coordinate system $\{y^i\}$ for the Hamilton–Jacobi equation

$$H = g^{ab}\partial_x a W \partial_x b W = E, \tag{4.33}$$

$g^{ij} = g^{ji}$, $1 \leqslant i,j \leqslant n$, are that there exist $n-1$ quadratic functions $A^{\alpha} = a^{(\alpha)ab} p_a p_b$ satisfying the following.

(1) The $\{A^{\alpha}\}$ are constants of the motion, i.e., $[H, A^{\alpha}] = 0$, $\alpha = 1,\ldots,n-1$, where $[\ ,\ ]$ is the Poisson bracket.

(2) The $\{A^{\alpha}\}$ are in involution: $[A^{\alpha}, A^{\beta}] = 0$, $1 \leqslant \alpha,\beta \leqslant n-1$.

(3) The set $\{H, A^1,\ldots,A^{n-1}\}$ is linear independent (as n quadratic forms).

(4) At least one of the quadratic forms, say A^1, has simple roots.

(5) In a local coordinate system $\{z^i\}$ the quadratic forms satisfy the algebraic commutation property

$$a^{(\alpha)}{}_{ab} a^{(\beta)b}{}_c = a^{(\beta)}{}_{ab} a^{(\alpha)b}{}_c.$$

To obtain additive separable solutions we identify

$p_x i = \partial_x i W$ and look for solutions of the form $W = \Sigma_{i=1}^{n} W_i(y^i, \mathbf{c})$, which are a complete integral, i.e., $\det(\partial_{y^i} \partial_{c_j} W) \neq 0$, $\mathbf{c} = (c_1, \ldots, c_n)$.

For oblate spheroidal coordinates a suitable choice of basis for the constants of the motion $\{A^{(\alpha)}\}$ is

$$A^1 = m_{23}^2 + m_{24}^2 + m_{34}^2 + a^2(p_2^2 + p_3^2), \quad A^1 = p_1^2, \quad A^3 = m_{23}^2. \tag{4.34}$$

Strictly speaking a set of constants of the motion in which A^1 is replaced by $\mathbb{D}$ will not satisfy the criteria of our theorem. In particular, condition (5) is not satisfied. However, it is obvious from (4.28) and (4.34) that in oblate spheroidal coordinates we could always choose separable solutions for which $D = c_1$, $p_1^2 = c_2$, $m_{23}^2 = c_3$, for fixed constants c_1, c_2, c_3. Thus there are involutive sets of operators that do not satisfy the criteria of our theorem but that admit additively separable solutions in which each element of this involutive set is a constant. Furthermore these involutive sets define different null tetrads from those defined for the involutive set satisfying the Theorem:

$$l^i = (1/\sqrt{2})(\tilde{e}_t^a + \tilde{e}_r^a),$$
$$n^i = (1/\sqrt{2})(\tilde{e}_t^a - \tilde{e}_r^a),$$
$$m^i = (1/\sqrt{2})(\tilde{e}_\theta^a + i\tilde{e}_\phi^a).$$

From the group-theoretic point of view it is not possible to use group motions under the adjoint action of the Lie algebra to transform the set $\{\mathbb{D}, p_1^2, m_{23}^2, H\}$ into $\{A^1, A^2, A^3, H\}$ as in (4.34). Thus if we classify orbits of triplets $\{L_1, L_2, L_2\}$ of second-order elements in the enveloping algebra (to within the addition of arbitrary multiples of H), the sets $\{\mathbb{D}, p_1^2, m_{23}^2\}$ and $\{A^1, A^2, A^3\}$ lie on different orbits. Although there is only one orbit that corresponds to the conditions of the theorem, there are, in general, several orbits of involutive sets of operators for which variable separation is possible in a fixed coordinate system. The analysis we have made of this specific case of separation of variables proceeds in an analogous way for the other two examples of variable separation we have given, viz. coordinates (4.16) and (4.23) and associated null tetrads (4.17) and (4.22), respectively. More recently Carter and McLenaghan[18] have given a master separation equation for all the separable perturbations of spin-0, -½, -1, and -2 in a Kerr space-time background. Kamran and McLenaghan[19] have also gone some way toward finding the conditions under which separation of variables occurs for the Dirac and neutral equations. It is our intention to pursue these matters further and develop an intrinsic theory of variable separation for equations of physical importance.

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PCT theorem for fields with arbitrary high-energy behavior

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A neutral scalar field $A(x)$ is considered that has to be smeared by Fourier transforms of C^∞ functions with compact support but otherwise fulfills all the Wightman axioms, except strict local commutativity. It is shown to fulfill the PCT symmetry condition (where Ω denotes the vacuum state vector) $\langle\Omega|A(x_1)\cdots A(x_n)\Omega\rangle = \langle\Omega|A(-x_n)\cdots A(-x_1)\Omega\rangle$ if and only if $\langle\Omega|A(x_1)\cdots A(x_n)\Omega\rangle - \langle\Omega|A(x_n)\cdots A(x_1)\Omega\rangle$ can be represented, in a sense, as an infinite sum of derivatives of measures with supports containing no Jost points.

I. INTRODUCTION

As pointed out in Ref. 1 it might be important in quantum field theory to avoid any *a priori* restriction on the high-energy behavior of the fields. Therefore the Schwartz space[2] $\mathcal{S}(\mathbf{R}^4)$ of standard Wightman theory[3] should be replaced by the Fourier dual $S^0(\mathbf{R}^4) = \tilde{\mathcal{D}}(\mathbf{R}^4)$ of $\mathcal{D}(\mathbf{R}^4)$. Obviously, this leads to a theory of highly nonlocalizable fields. Nevertheless, using a natural *relaxed locality condition*[4] it was possible to prove the spin-statistics theorem for such fields.[1]

The main purpose of the present paper is to derive the PCT symmetry within the same framework along the lines sketched in Ref. 4. In Sec. II we briefly review the notion of *quasisupport*, necessary for formulating the relaxed locality condition, and restate the basic conjecture made in Ref. 4. In Sec. III the corresponding form of the PCT theorem will be proved, assuming the basic conjecture to be correct. In Sec. IV, finally, the conjecture will be rigorously justified.

II. QUASISUPPORTS

As in Ref. 4, lacking any sensible notion of support for functionals on $S^0(\mathbf{R}^n) = \tilde{\mathcal{D}}(\mathbf{R}^n)$, let us introduce the following definition.

Definition[5]: A closed subset M of $\mathbf{R}^n$ is called a quasisupport of the generalized function $F \in S^0(\mathbf{R}^n)'$ iff, for every $\epsilon > 0$, there are complex-valued Borel measures $\mu_\alpha(\chi)$ on $\mathbf{R}^n$, $\alpha \in \mathbf{Z}_+^n$, with $\operatorname{supp}\mu_\alpha \subset U_\epsilon(M)$ and a function $N(A)$ on $\mathbf{R}^n$ such that

$$\sup_{\alpha\in\mathbf{Z}_+^n} A^{|\alpha|}\int |(1+\|\chi\|)^{-N(A)}\, d\mu_\alpha(\chi)| < \infty,$$

for every $A > 0$,

and

$$F(\chi) = \sum_{\alpha\in\mathbf{Z}_+^n} D_\chi^\alpha \mu_\alpha(\chi)$$

in the distributional sense.

Note that, according to Lemma 2.1 of Ref. 1, $M = \bar{M}$ is a quasisupport of $F \in S^0(\mathbf{R}^n)'$ if and only if F is locally continuous on M with respect to $S^0(\mathbf{R}^n)$ in the sense of Ref. 6. Therefore, an important consequence of Lemma 2.2 of Ref. 1 is the following lemma.

Lemma 1: Let $\epsilon > 0$ and $M \subset \mathbf{R}^n$. If $\overline{U_\epsilon(M)}$ is a quasisupport of $F \in S^0(\mathbf{R}^n)'$, then so is $\bar{M}$.

One of the essential tools used in the next section is the generalized nuclear theorem (Ref. 6, Lemma 2) for $S^0(\mathbf{R}^n)$. Let us, therefore, recall it in a form using the notion of essential support instead of local continuity.

Lemma 2: Let $(\phi_1,\ldots,\phi_n) \to F_0(\phi_1,\ldots,\phi_n)$ be a multilinear functional on $S^0(\mathbf{R}^1)\times\cdots\times S^0(\mathbf{R}^1)$ that is continuous in each variable separately. Then there is a unique generalized function $F \in S^0(\mathbf{R}^n)'$ fulfilling

$$F_0(\phi_1,\ldots,\phi_n) = \int d\chi\, F(\chi)\phi_1(\chi^1)\cdots\phi_n(\chi^n),$$

for $\phi_1,\ldots,\phi_n \in S^0(\mathbf{R}^1)$. Moreover, let $n' < n$ and let $M = \bar{M} \subset R^{n'}$. If, for arbitrary $\psi_{n'+1},\ldots,\psi_n \in S^0(\mathbf{R}^1)$, M is a quasisupport of the $S^0(\mathbf{R}^{n'})'$ element

$$\phi \to \int d\chi\, F(\chi)\phi(\chi^1,\ldots,\chi^{n'})\psi_{n'+1}(\chi^{n'+1})\cdots\psi_n(\chi^n),$$

then $M \times \mathbf{R}^{n-n'}$ is a quasisupport of $F \in S^0(\mathbf{R}^n)'$.

We conclude this section by reformulating[7] the basic conjecture made in Ref. 4.

Conjecture: Let the complement $\mathbf{R}^{4(n+1)} \setminus J_{n+1}$ of the set of Jost points

$$J_{n+1} \equiv \left\{\hat{x} \in \mathbf{R}^{4(n+1)} : \left(\sum_{\nu=1}^{n} \lambda_\nu (x_\nu - x_{\nu+1})\right)^2 < 0, \text{ for } \lambda_1,\ldots,\lambda_n \geq 0, \text{ with } \sum_{\lambda=1}^{n}\lambda_\nu > 0\right\}$$

be a quasisupport of $F \in S^0(\mathbf{R}^{4(n+1)})'$. If

$$\operatorname{supp}\tilde{F} \subset M_{n+1} \equiv \left\{\hat{p} \in \mathbf{R}^{4(n+1)} : p_1 + \cdots + p_{n+1} = 0,\ \sum_{\mu=1}^{\nu} p_\mu \in \overline{V_+}, \text{ for } \nu = 1,\ldots,n\right\},$$

then $F = 0$.

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By Lemma 1, this formulation is equivalent to the one presented in Ref. 4, indeed.

III. PCT THEOREM

As indicated in the Introduction, we consider a general field theory fitting into the Wightman framework (Ref. 3, Chap. 3) subject to the following two modifications.

Modification 1: Replace $\mathscr{S}(\mathbf{R}^4)$ by $S^0(\mathbf{R}^4)$.

Modification 2: Relax the usual locality condition by using the notion of quasisupport.

For simplicity we deal with a single neutral scalar field $A(x)$, only.

By Lemma 2 the $(n+1)$-point function

$$\mathscr{W}(\hat{x}) \equiv \langle \Omega | A(x_1) \cdots A(x_{n+1}) \Omega \rangle \in S^0(\mathbf{R}^{4(n+1)})'$$

has the following property.

Essential weak locality: $\mathbf{R}^{4(n+1)} \setminus J_{n+1}$ is a quasisupport of

$$\mathscr{W}(x_1,\ldots,x_{n+1}) - \mathscr{W}(x_{n+1},\ldots,x_1) \in S^0(\mathbf{R}^{4(n+1)})'.$$

We want to prove that essential weak locality is equivalent to the following property.

PCT symmetry:

$$\mathscr{W}(x_1,\ldots,x_{n+1}) = \mathscr{W}(-x_{n+1},\ldots,-x_1).$$

The idea, of course, will be to apply the conjecture of Sec. II to

$$F(\hat{x}) \equiv \mathscr{W}(x_1,\ldots,x_{n+1}) - \mathscr{W}(-x_{n+1},\ldots,-x_1)$$

in order to get PCT symmetry from essential weak locality.

Indeed, as in standard Wightman theory (Ref. 3, Theorem 3.2), we easily check

$$\operatorname{supp} \tilde{\mathscr{W}}(\hat{p}) \subset M_{n+1},$$

hence also

$$\operatorname{supp} \tilde{F}(\hat{p}) \subset M_{n+1}.$$

Therefore, we are left to prove that $\mathbf{R}^{4(n+1)} \setminus J_{n+1}$ is a quasisupport of $F(\hat{x})$ if and only if essential weak locality holds. The latter equivalence is a direct consequence of the following lemma.

Lemma 3: $\mathbf{R}^{4(n+1)} \setminus J_{n+1}$ is a quasisupport of the generalized function $\mathscr{W}(\hat{x}) - \mathscr{W}(-\hat{x}) \in S^0(\mathbf{R}^{4(n+1)})'$.

Proof of Lemma 3: As in standard Wightman theory (Ref. 3, Chap. 2.1) we easily see that there is a Lorentz-invariant generalized function[8] $W(\hat{\xi}) \in S^0(\mathbf{R}^{4n})'$ fulfulling

$$\int d\hat{\xi}\, W(\pm\hat{\xi}) \int dx_{n+1}\, \psi(\hat{\xi}, x_{n+1}) = \int d\hat{x}\, \mathscr{W}(\pm\hat{x}) \psi(x_1 - x_2,\ldots,x_n - x_{n+1}, x_{n+1}), \quad \text{for } \psi \in S^0(\mathbf{R}^{4(n+1)}) \tag{3.1}$$

and

$$\operatorname{supp} \tilde{W} \subset \overline{V_+} \times \cdots \times \overline{V_+}. \tag{3.2}$$

Now (3.1), Lemma 2, and an elementary estimate show that $\mathbf{R}^{4(n+1)} \setminus J_{n+1}$ is a quasisupport of

$$\mathscr{W}(\hat{x}) - \mathscr{W}(-\hat{x}) \in S^0(\mathbf{R}^{4(n+1)})'$$

if $\mathbf{R}^{4n} \setminus \hat{J}_n$, where

$$\hat{J}_n \equiv \left\{ \hat{\xi} \in \mathbf{R}^{4n} : \left(\sum_{\nu=1}^{n} \lambda_\nu \xi_\nu \right)^2 < 0, \text{ for } \lambda_1,\ldots,\lambda_n \geqslant 0, \text{ with } \sum_{\nu=1}^{n} \lambda_\nu > 0 \right\}$$

is a quasisupport of $W(\hat{\xi}) - W(-\hat{\xi}) \in S^0(\mathbf{R}^{4n})'$. Thus, by Ref. 1, Lemma 2.1, it is sufficient to prove that

$$\sup_{\phi \in S} \left| \int d\hat{\xi} (W(\hat{\xi}) - W(-\hat{\xi})) \phi(\hat{\xi}) \right| < \infty, \tag{3.3}$$

for every subset S of $S^0(\mathbf{R}^{4n})$ that is locally bounded on $\mathbf{R}^{4n} \setminus \hat{J}_n$. Local boundedness in the present case means existence of some $\epsilon > 0$ such that

$$\sup_{\phi \in S} \sup_{\hat{\xi} \in U_\epsilon(\mathbf{R}^{4n} \setminus \hat{J}_n)} \sup_{\hat{\alpha} \in \mathbf{Z}_+^{4n}} (1 + \|\hat{\xi}\|)^N \epsilon^{|\hat{\alpha}|} |D_{\hat{\xi}}^{\hat{\alpha}} \phi(\hat{\xi})| < \infty, \tag{3.4}$$

for every positive integer N. By Lemma 2.2 of Ref. 1, (3.4) implies

$$\sup_{\xi^0_1,\ldots,\xi^0_n \in \mathbf{R}^1} \sup_{\alpha^0_1,\ldots,\alpha^0_n \in \mathbf{Z}_+} (1 + \|\hat{\xi}\|)^N \epsilon^{\alpha^0_1 + \cdots + \alpha^0_n} \times \left| \left(\frac{\partial}{\partial \xi^0_1} \right)^{\alpha^0_1} \cdots \left(\frac{\partial}{\partial \xi^0_n} \right)^{\alpha^0_n} \phi(\hat{\xi}) \right| < \infty, \quad \text{for } \phi \in S,\ (\xi^1_1,\ldots,\xi^3_n) \in \mathbf{R}^{3n},\ N = 1,2,\ldots,$$

and hence

$$\operatorname{supp} \tilde{\phi} \subset \{ \hat{q} \in \mathbf{R}^{4n} : |q^0_\nu| \leqslant 1/\epsilon, \text{ for } \nu = 1,\ldots,n \}, \quad \text{for } \phi \in S. \tag{3.5}$$

We now choose some $g \in \mathscr{D}(\mathbf{R}^1)$ fulfilling

$$g(t) = 1, \quad \text{if } |t| \leqslant (n/\epsilon)^2, \tag{3.6}$$

and define

$$\tilde{W}_g(\hat{q}) \equiv \tilde{W}(\hat{q}) g((q_1 + \cdots + q_n)^2).$$

Then (3.2), (3.5), and (3.6) imply

$$\int d\hat{\xi} (W(\hat{\xi}) - W(-\hat{\xi})) \phi(\hat{\xi}) = \int d\hat{\xi} (W_g(\hat{\xi}) - W_g(-\hat{\xi})) \phi(\hat{\xi}), \quad \text{for } \phi \in S. \tag{3.7}$$

On the other hand, since g has compact support and since $W(\hat{\xi})$ is Lorentz invariant, we easily see[9] that $W_g(\hat{\xi})$ is [the restriction to $S^0(\mathbf{R}^{4n})$ of] a *tempered* Lorentz invariant distribution. Moreover, (3.2) implies

$$\operatorname{supp} \tilde{W}_g \subset \overline{V_+} \times \cdots \times \overline{V_+}.$$

Therefore, we may apply the standard BHW technique (Ref. 10, Part I) to obtain

$$\operatorname{supp}(W_g(\hat{\xi}) - W_g(-\hat{\xi})) \subset \mathbf{R}^{4n} \setminus \hat{J}_n.$$

This together with (3.7) and (3.4) implies what we were left to prove, namely, (3.3). ∎

Summarizing, assuming the conjecture of Sec. II to be correct, we have proved the following theorem.

PCT Theorem: Let the neutral scalar field $A(x)$ fulfill all the Wightman axioms, except locality, with $\mathscr{S}(\mathbf{R}^4)$ replaced by $S^0(\mathbf{R}^4)$. Then PCT symmetry is equivalent to essential weak locality, as defined above.

IV. PROOF OF THE BASIC CONJECTURE

Let $F \in S^0(\mathbf{R}^{4(n+1)})'$ fulfill the requirements of the conjecture of Sec. II. Then, by Lemma 2, it is sufficient to prove[11]

$$G_\phi(\hat{\xi}) = 0, \quad \text{for every } \phi \in S^0(\mathbf{R}^{2n+4}),$$

where $G_\phi(\hat{\xi}) \in S^0(\mathbf{R}^{2n})'$ is defined by

$$\int d\hat{\xi}\, G_\phi(\hat{\xi})\psi(\hat{\xi}) \equiv \int d\hat{x}\, F(\hat{x})\psi(x_1^0 - x_2^0, x_1^1 - x_2^1, \ldots, x_n^0 - x_{n+1}^0, x_n^1 - x_{n+1}^1)$$
$$\times \phi(x_1^2 - x_2^2, x_1^3 - x_2^3, \ldots, x_n^2 - x_{n+1}^2, x_n^3 - x_{n+1}^3, x_{n+1}),$$

for $\psi \in S^0(\mathbf{R}^{2n})$. Let us define

$$V_1 \equiv \{\xi \in \mathbf{R}^2 : \xi^0 > |\xi^1|\}, \quad V_2 \equiv \{\xi \in \mathbf{R}^2 : \xi^1 > |\xi^0|\}, \quad V_3 \equiv \{\xi \in \mathbf{R}^2 : -\xi^0 > |\xi^1|\}, \quad V_4 \equiv \{\xi \in \mathbf{R}^2 : -\xi^1 > |\xi^0|\}.$$

Then, for $\phi \in S^0(\mathbf{R}^{2n+4})$, one easily checks that $\mathbf{R}^{2n} \setminus \hat{J}_n^{(2)}$, where

$$\hat{J}_n^{(2)} \equiv \{\hat{\xi} \in \mathbf{R}^{2n} : \text{either } \xi_\nu \in V_2 \quad \text{for } \nu = 1,\ldots,n \text{ or } \xi_\nu \in V_4 \text{ for } \nu = 1,\ldots,n\},$$

is a quasisupport of $G_\phi \in S^0(\mathbf{R}^{2n})'$ and that[12]

$$\operatorname{supp} \tilde{G}_\phi \subset \overline{V_1} \times \cdots \times \overline{V_1}.$$

Therefore it is sufficient to prove the following theorem.

Auxiliary Theorem: Let $\mathbf{R}^{2n} \setminus \hat{J}_n^{(2)}$ be a quasisupport of $G \in S^0(\mathbf{R}^{2n})'$. If $\operatorname{supp} \tilde{G} \subset \overline{V_1} \times \cdots \times \overline{V_1}$, then $G = 0$.

Unfortunately, there seems to be no simple way of reducing the general case $n > 1$ to the special case $n = 1$, managed in Ref. 1. This is because the spaces $S^0(\mathbf{R}^k)$ do not contain functions with exponential decrease at infinity.

In the course of the proof of the auxiliary theorem we shall use the following notation:

$$\mathcal{J} \equiv \{j = (j^1,\ldots,j^n) : j^\nu \in \{1,2,3,4\}, \text{ for } \nu = 1,\ldots,n \text{ and } j \neq (22,\ldots,2), (4,4,\ldots,4)\},$$

$$\mathcal{V}_j \equiv \overline{V_{j^1}} \times \cdots \times \overline{V_{j^n}}, \quad \text{for } j \in \mathcal{J},$$

$$\Gamma_j \equiv (\mathbf{R}^2 + iV_{j^1}) \times \cdots \times (\mathbf{R}^2 + iV_{j^n}), \quad \text{for } j \in \mathcal{J},$$

$$d(\delta) \equiv (\delta \cos(\pi/2 - \delta))^{-1}, \quad \text{for } \delta \in (0,\pi),$$

$$\left.\begin{aligned} B_{1,\delta} &\equiv \{\eta \in \mathbf{R}^2 : |\eta^1| < \eta^0 \tan(\pi/4 - \delta),\ \|\eta\| < d(\delta)\},\\ B_{2,\delta} &\equiv \{\eta \in \mathbf{R}^2 : (\eta^1, \eta^0) \in B_{1,\delta}\},\\ B_{3,\delta} &\equiv -B_{1,\delta}, \quad B_{4,\delta} \equiv -B_{2,\delta}, \end{aligned}\right\} \text{ for } \delta \in (0,\pi/4),$$

$$\Gamma_{j,\delta} \equiv (\mathbf{R}^2 + iB_{j^1,\delta}) \times \cdots \times (\mathbf{R}^2 + iB_{j^n,\delta}), \quad \text{for } j \in \mathcal{J} \text{ and } \delta \in (0,\pi/4).$$

By straightforward generalization[13] of the auxiliary results presented in Lücke[13] we get the following lemma and corollary.

Lemma 4: For sufficiently small $\delta > 0$, the region

$$\{q + i\eta \in \mathbf{C}^2 : \|q\| + \|\eta\| < n\}$$

is contained in the envelope of holomorphy of

$$(\mathbf{R}^2 \setminus \overline{V_1}) \cup (\mathbf{R}^2 + iB_{1,\delta}) \cup (\mathbf{R}^2 + iB_{3,\delta}).$$

Corollary: Let $\delta > 0$ be sufficiently small and let f be a polynomially bounded function over $\mathbf{R}^2$ fulfilling

$$\sup_{\lambda \in \mathbf{R}^1} \sup_{a \in B_{2,\delta}} \exp(\|\lambda a\|/\delta)\, |f(\lambda a)| < \infty.$$

If $\operatorname{supp} \tilde{f} \subset \overline{V_1}$, then $\tilde{f}(q) = 0$, for $q \in U_n^{(2)}(0) \equiv \{q \in \mathbf{R}^2 : \|q\| < n\}$.

Now we are well prepared for the proof.

Proof of the auxiliary theorem: Given arbitrary $N > 0$ and $\tilde{\chi} \in \mathcal{D}(\mathbf{R}^{2n})$ fulfilling

$$\operatorname{supp} \tilde{\chi} \subset V_1 \times \cdots \times V_1, \tag{4.1}$$

it is obviously sufficient to prove[14]

$$(\tilde{G} * \tilde{\chi})(\hat{q}) = 0, \quad \text{if } \|q_\nu\| < N, \quad \text{for } \nu = 1,\ldots,n. \tag{4.2}$$

Since $\cup_{j \in \mathcal{J}} \mathcal{V}_j$ is a quasisupport of G, we may represent G as a sum

$$G = \sum_{j \in \mathcal{J}} G_j, \tag{4.3}$$

where $\mathcal{V}_j$ is a quasisupport of $G_j \in S^0(\mathbf{R}^{2n})'$ for $j \in \mathcal{J}$. Therefore the Laplace transform[15] $\mathcal{L}G_j$ of $G_j, j \in \mathcal{J}$, may be defined as an analytic function over Γ_j fulfilling

$$\lim_{\epsilon\to 0}\sup_{\substack{\hat{q}+i\hat{\eta}\in\Gamma_j\\ \hat{q}\in K,\|\eta\|<\epsilon}}\left|(\tilde{G}_j{}^{*}\tilde{\chi})(\hat{q})-\int d\hat{q}'(\mathscr{L}G_j)(\hat{q}'+i\hat{\eta})\tilde{\chi}(\hat{q}-\hat{q}')\right|=0,\quad\text{for every compact subset } K \text{ of } \mathbf{R}^{2n}. \tag{4.4}$$

Let us now choose some $\delta\in(0,\pi/4)$, being sufficiently small in the sense of the corollary, and two bounded analytic functions $h^0(q)$, $h^1(q)$ over $\mathbf{R}^2+iU^{(2)}_{d(\delta/3)}(0)$ fulfilling, there, the conditions[16]

$$\begin{aligned} &q\in V_k\Rightarrow h(q)\equiv(h^0(q),h^1(q))\in V_k,\\ &\eta\in V_k\Rightarrow h(q+i\eta)\in\mathbf{R}^2+iV_k, \end{aligned} \tag{4.5}$$

for $k=1,2,3,4$,

$$U^{(2)}_N(0)\subset h(U^{(2)}_1(0)), \tag{4.6}$$

and

$$\lim_{\epsilon\to 0}\sup_{q+i\eta\in\mathbf{R}^2+iU^{(2)}_\epsilon(0)}\|\mathrm{Im}\,h(q+i\eta)\|=0.$$

Thus, for $j\in\mathscr{J}$,

$$\begin{aligned}&\tilde{H}_j(\hat{q}+i\hat{\eta})\\ &\equiv\int d\hat{q}'\,(\mathscr{L}G_j)\\ &\quad\times((h(q_1+i\eta_1),\ldots,h(q_n+i\eta_n))-\hat{q}')\chi(\hat{q}')\end{aligned}$$

is bounded and analytic over $\Gamma_{j,\delta/3}$ and, by (4.4), fulfills

$$\lim_{\epsilon\to 0}\sup_{\substack{\hat{q}+i\hat{\eta}\in\Gamma_{j,\delta/3}\\ \|\hat{\eta}\|<\epsilon}}|\tilde{H}_j(\hat{q})-\tilde{H}_j(\hat{q}+i\hat{\eta})|=0, \tag{4.7}$$

where

$$\tilde{H}_j(\hat{q})\equiv(\tilde{G}_j{}^{*}\tilde{\chi})(h(q_1),\ldots,h(q_n)),\quad\text{for }\hat{q}\in\mathbf{R}^{2n}. \tag{4.8}$$

Next, define

$$\begin{aligned}f_j(a,\hat{\xi})\equiv&\int d\hat{q}\,\tilde{H}_j(\hat{q})\exp\left(-\sum_{\nu=1}^{n}\|q_\nu\|^2\right)\\ &\times\exp\left(-i\sum_{\nu=1}^{n}q_\nu\cdot(\xi_\nu-a)\right),\end{aligned} \tag{4.9}$$

for $a\in\mathbf{R}^2$ and $\hat{\xi}\in\mathbf{R}^{2n}$. Then, by (4.7) together with boundedness and analyticity of $\tilde{H}_j$, the Cauchy integral theorem implies

$$\begin{aligned}f_j(a,\hat{\xi})=&\int d\hat{q}\,\tilde{H}_j(\hat{q}+i\hat{\eta})\exp(-(\hat{q}+i\hat{\eta})^2)\\ &\times\exp\left(-i\sum_{\nu=1}^{n}q_\nu\cdot(\xi_\nu-a)\right)\\ &\times\exp\left(\hat{\eta}\cdot\hat{\xi}-a\cdot\sum_{\nu=1}^{n}\eta_\nu\right),\\ &\text{for }\hat{\xi}+i\hat{\eta}\in\Gamma_{j,\delta/3}.\end{aligned} \tag{4.10}$$

For every $j\in\mathscr{J}$ there is some $\nu_0\in\{1,\ldots,n\}$ with $j^{\nu_0}\neq 4$ and some $\eta_{\nu_0}\in B_{j^{\nu_0},\delta/3}$ with

$$\inf_{a\in B_{2,\delta}}\frac{a}{\|a\|}\cdot\frac{\eta_{\nu_0}}{\|\eta_{\nu_0}\|}>\cos\left(\frac{\pi}{2}-\frac{\delta}{2}\right).$$

Hence, choosing $\|\eta_{\nu_0}\|$ sufficiently large and $\|\eta_\nu\|$ for $\nu\neq\nu_0$ sufficiently small in (4.10), we see that

$$\sup_{\lambda>0}\sup_{a\in B_{2,\delta}}\exp(\|\lambda a\|/\delta)\,|f_j(\lambda a,\hat{\xi})|<\infty,$$

for $j\in\mathscr{J}$ and $\hat{\xi}\in\mathbf{R}^{2n}$. Similarly,

$$\sup_{\lambda>0}\sup_{a\in B_{4,\delta}}\exp(\|\lambda a\|/\delta)\,|f_j(\lambda a,\hat{\xi})|<\infty.$$

Summing over j we get

$$\sup_{\lambda\in\mathbf{R}^1}\sup_{a\in B_{2,\delta}}\exp(\|\lambda a\|/\delta)\,|f_{\hat{\xi}}(\lambda a)|<\infty, \tag{4.11}$$

for $\hat{\xi}\in\mathbf{R}^{2n}$, where

$$f_{\hat{\xi}}(a)\equiv\sum_{j\in\mathscr{J}}f_j(-a,\hat{\xi}),\quad\text{for } a\in\mathbf{R}^2,\quad\hat{\xi}\in\mathbf{R}^{2n}.$$

Equations (4.9), (4.8), and (4.3) imply

$$\begin{aligned}f_{\hat{\xi}}(a)=&\int d\hat{q}(\tilde{G}^{*}\tilde{\chi})(h(q_1,\ldots,h(q_n))\\ &\times\exp\left(-\sum_{\nu=1}^{n}\|q_\nu\|^2\right)\exp\left(-i\sum_{\nu=1}^{n}q_\nu(\xi_\nu+a)\right).\end{aligned} \tag{4.12}$$

Therefore, by (4.1) and (4.5) we have

$$\mathrm{supp}\,f_{\hat{\xi}}\subset\overline{V_1},$$

since

$$\mathrm{supp}\,\tilde{G}\subset\overline{V_1}\times\cdots\times\overline{V_1}.$$

This together with (4.11) implies

$$f_{\hat{\xi}}(q)=0,\quad\text{for } q\in U^{(2)}_n(0),$$

by the corollary. Thus, integrating (4.12) with suitable test functions of a and $\hat{\xi}$, we see

$$\begin{aligned}&(\tilde{G}^{*}\tilde{\chi})(h(q_1),\ldots,h(q_n))=0,\\ &\quad\text{if }\|q_\nu\|<1,\quad\text{for }\nu=1,\ldots,n.\end{aligned}$$

By (4.6), this implies (4.2), completing the proof of the auxiliary theorem. ■

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I am indebted to Professor H. D. Doebner for support and encouragement.

[1] W. Lücke, "Spin-statistics theorem for fields with arbitrary high energy behavior," Acta Phys. Austr. **55**, 213 (1984).

[2] We use Schwartz's [L. Schwartz, *Théorie des distributions* (Hermann, Paris, 1966)] standard notation for test spaces.

[3] R. F. Streater and A. S. Wightman, *PCT, Spin and Statistics, and All That* (Benjamin, New York, 1964).

[4] W. Lücke, "On possible relaxations of strict locality in relativistic quantum field theory," talk presented at the Conference on Differential Geometric Methods in Theoretical Physics, Shumen, Bulgaria, 20–25 August, 1984.

[5] We use standard notation: $S^0(\mathbf{R}^n)'$ denotes the topological dual of $S^0(\mathbf{R}^n)$, $U_\epsilon(M)$ the ϵ neighborhood of M, $\overline{M}$ the closure of M, and $\mathbf{Z}_+$ the set of non-negative integers. For $\alpha=(\alpha^1,\ldots,\alpha^n)\in\mathbf{Z}^n_+=\mathbf{Z}_+\times\cdots\times\mathbf{Z}_+$ and $\chi=(\chi^1,\ldots,\chi^n)\in\mathbf{R}^n$, we write

$$|\alpha| \equiv \alpha^1 + \cdots + \alpha^n, \quad D_\chi^\alpha \equiv \left(\frac{\partial}{\partial \chi^1}\right)^{\alpha^1} \cdots \left(\frac{\partial}{\partial \chi^n}\right)^{\alpha^n},$$

$$\|\chi\| \equiv + \sqrt{(\chi^1)^2 + \cdots + (\chi^n)^2}.$$

[6]J. Bümmerstede and W. Lücke, "Haag–Ruelle–Hepp scattering formalism for essentially local non-local fields," Commun. Math. Phys. **37**, 121 (1974).

[7]Here and in the next section we write $\hat{x}$ for $(x_1,\ldots,x_{n+1})$ [resp. $\hat{p}$ for $(\hat{p}_1,\ldots,\hat{p}_{n+1})$], where $x_\nu = (x_\nu^0, x_\nu^1, x_\nu^2, x_\nu^3) \in \mathbf{R}^4$ [resp. $p_\nu = (p_\nu^0, p_\nu^1, p_\nu^2, p_\nu^3) \in \mathbf{R}^4$], for $\nu = 1,\ldots,n+1$. Here $\tilde{F}$ denotes the Fourier transform of F:

$$\tilde{F}(\hat{p}) \equiv (2\pi)^{-2(n+1)} \int d\hat{x}\, F(\hat{x}) \exp(i\hat{x} \cdot \hat{p}),$$

$$\hat{x} \cdot \hat{p} \equiv x_1 \cdot p_1 + \cdots + x_{n+1} \cdot p_{n+1},$$

$$x_\nu \cdot p_\nu \equiv x_\nu^0 p_\nu^0 - x_\nu^1 p_\nu^1 - x_\nu^2 p_\nu^2 - x_\nu^3 p_\nu^3.$$

Here V_+ denotes the open future light cone.

[8]We write $\hat{\xi}$ for $(x_1 - x_2,\ldots,x_n - x_{n+1}) \in \mathbf{R}^{4n}$ and $\hat{q}$ for $(q_1,\ldots,q_n)$, where $q_\nu = (q_\nu^0, q_\nu^1, q_\nu^2, q_\nu^3) \in \mathbf{R}^4$, for $\nu = 1,\ldots,n$.

[9]Compare J. Bümmerstede and W. Lücke, "The notion of essential locality for nonlocalizable fields," J. Math. Phys. **16**, 1203 (1975), Lemma 2 or W. Lücke, "Eine allgemeine Theorie nicht notwendig lokalisierbarer relativistischer Quantenfelder," Habilitationsschrift, Clausthal, 1978, Lemma II.2.

[10]H. Araki, "Wightman functions, retarded functions and their analytic continuations," Prog. Theor. Phys. (Kyoto) Suppl. **18**, 83 (1961).

[11]In this section, we still write $\hat{\xi}$ for $(\xi_1,\ldots,\xi_n)$, $\hat{q}$ for $(q_1,\ldots,q_n)$, etc., and $\hat{\xi} \cdot \hat{q}$ for $\xi_1 \cdot q_1 + \cdots + \xi_n \cdot q_n$. However, now $\xi_\nu = (\xi_\nu^0, \xi_\nu^1) \in \mathbf{R}^2$, $q_\nu = (q_\nu^0, q_\nu^1) \in \mathbf{R}^2$, etc., and $\xi_\nu \cdot q_\nu = \xi_\nu^0 q_\nu^0 + \xi_\nu^1 q_\nu^1$, for $\nu = 1,\ldots,n$. Occasionally, the *Euclidean* inner products, now also used for Fourier transformation, are applied to complex vectors, meaning analytic continuation.

[12]Actually, we do not need the property $p_1 + \cdots + p_{n+1} = 0$ for $\hat{p} \in \operatorname{supp} \tilde{F}$.

[13]We just have to restrict to $|\omega_0|, |\omega_1| < N^2$ in W. Lücke, "PCT, spin and statistics, and all that for nonlocal Wightman fields," Commun. Math. Phys. **65**, 77 (1979), Sec. 2, and use Lemma 1 of H. Epstein, "Some analytic properties of scattering amplitudes in quantum field theory," in *Axiomatic Field Theory*, edited by M. Chrétien and S. Deser (Gordon and Breach, New York, 1966), Sec. II. 4.4.

[14]$\tilde{G} * \tilde{\chi}$ denotes the convolution product of $\tilde{G}$ and $\tilde{\chi}$.

[15]Compare Ref. 1, proof of Theorem 4.

[16]For instance (compare Epstein,[13] p. 57), we may choose

$$h^0(q) = \tau^2 \left(\tanh \frac{q^0 + q^1}{\tau} + \tanh \frac{q^0 - q^1}{\tau} \right),$$

$$h^1(q) = \tau^2 \left(\tanh \frac{q^0 + q^1}{\tau} - \tanh \frac{q^0 - q^1}{\tau} \right),$$

with sufficiently large $\tau > 0$.

Simple waves for equation of potential, nonstationary flow of compressible gas

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Certain classes of the exact solution of the equation of nonstationary potential flow of a compressible gas are found. The method described by Kalinowski [M. W. Kalinowski, J. Math. Phys. **25**, 2620 (1984); Lett. Math. Phys. **6**, 17 (1983); **7**, 479 (1983)] is applied. These considerations are carried out locally at an established point of space of a hodograph. Some algebraic properties of simple integral elements are analyzed, and certain exact classes of solutions are constructed. Finally a certain physical analysis of the achieved results is carried out.

I. INTRODUCTION

Let us consider the system of partial differential equations of the form

$$a_j^{s\nu}(u^1,u^2,...,u^l)\frac{\partial u_j}{\partial x^\nu}(x^1,x^2,...,x^n)=0, \quad (1)$$

$$s=1,...,m, \quad \nu=1,...,n$$

$$j=1,...,l, \quad m\geqslant l,$$

$$x=(x^1,x^2,...,x^n)\in E,$$

$$u(x)=(u^1(x),...,u^l(x))\in H,$$

which is a quasilinear, homogeneous system of the first order with coefficients dependent only on the unknown functions.

This system may be undetermined, i.e., $m\geqslant l$. Let us assume that this system is nonelliptical. That means that there are nontrivial solutions of the algebraic system of equations

$$a_j^{s\nu}\gamma^j\lambda_l=0, \quad \text{where } \operatorname{rank}\|a_j^{s\nu}\lambda_\nu\|<l, \quad (2)$$

for the vectors $\gamma\in R^l$ and $\lambda\in R^n$. The above algebraic system of equations defines the so-called knotted characteristic vectors respectively in a hodograph space $H=R^l$ (space of values of the unknown functions) and in physical space $E=R^n$ (independent variables). The pair γ and λ is called knotted, if it satisfies Eq. (2). This fact is denoted by $\gamma\sim\lambda$. Matrix $L_\nu^j=\gamma^j\cdot\lambda_\nu$ created by the pair of knotted vectors is called a simple integral element since $\operatorname{rank}\|L_\nu^j(u_0)\|=1$. It is convenient to treat λ as an element of space E^*. On the other hand, in the terminology of tensor calculus, if we consider $x\in E$ as a contravariant vector then $\lambda\in E^*$ is a covariant vector. In this language element L is an element of tensor space $T_uH\otimes E^*$ of the form $L=\nu\otimes\lambda$.

Now we introduce the concept of a simple wave, which provides us with the separation of simple integral elements from the set of integral elements. Let the map u: $D\to H$, $D\subset E$ be any solution of system (1). We call it a simple wave for a homogeneous system if the tangent mapping du is a simple element at any point $x_0\in D$. Let us consider the smooth curve Γ: $u=f(R)$ in the hodograph space H parametrized by R, such that the tangent vector

$$\frac{df(R)}{dR}=\gamma(f(R)) \quad (3)$$

is a characteristic vector. Then, there exists a field of the characteristic covectors $\lambda(u)$, connected with the field $\gamma(f(R))$, defined on the curve Γ: $\lambda=\lambda(f(R))$. We have the following theorem.

The Theorem: If the curve $\Gamma\subset H$ obeys the condition (3) and if $\phi(\cdot)$ is a differentiable function of one variable, then the function $u=u(x)$ given in an implicit way by the relations

$$u=f(R), \quad R=\phi(\lambda_\nu(f(R))x^\nu),$$
$$a_j^{s\nu}\gamma^j\lambda_\nu=0, \quad (4)$$

is the solution of the basic system (1). The above solution is called a simple wave (or the Riemann wave). The proof may be obtained by direct differentiation of the relations (4). Vector λ appearing in this expression defines velocity and a direction of appropagation of waves. The curve Γ obeying the condition (3) is called a characteristic curve in the hodograph space. This theorem tells us that if the map u: $E\subset D\to H$ is a simple wave then the image of map u is a characteristic curve in space H. A parameter R defined on this curve is called the Riemann invariant.

II. EQUATION OF POTENTIAL FLOW OF COMPRESSIBLE GAS

In this paper we discuss the flat nonstationary flow of compressible gas described by potential of velocity and density

$$\ln\rho=-\Phi_{,t}, \quad \mathbf{v}=\nabla\Phi. \quad (5)$$

This assumption allows us to describe discontinuities of velocity and density as a change of the gauge of this potential on both sides of the surface of discontinuity. Eliminating density ρ from the mass conservation law,

$$\frac{\partial\rho}{\partial t}+\operatorname{div}(\rho\mathbf{v})\equiv\left(\frac{\partial}{\partial t}+\mathbf{v}\nabla\right)\rho+\rho\operatorname{div}\mathbf{v}=0,$$

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by means of the Euler equation

$$\left(\frac{\partial}{\partial t}+\mathbf{v}\nabla\right)\mathbf{v}=-\frac{\nabla p}{\rho}=-\frac{c^2}{\rho}\nabla\rho,$$

we get

$$\frac{\partial \ln\rho}{\partial t}+c^2\,\mathrm{div}\,\mathbf{v}-\mathbf{v}\left(\frac{\partial \mathbf{v}}{\partial t}+(\mathbf{v}\nabla)\mathbf{v}\right)=0.$$

Introducing here the potential according to Eq. (5) we find[1-3]

$$\Phi_{,tt}+2(\Phi_{,x}\Phi_{,xt}+\Phi_{,y}\Phi_{,yt})+2\Phi_{,x}\Phi_{,y}\Phi_{,xy}+(\Phi_{,x}^2-c^2)\Phi_{,xx}+(\Phi_{,y}^2-c^2)\Phi_{,yy}=0, \tag{6}$$

where the lowest indices are for partial derivatives. The velocity of sound C^2 is given by a variant of the (compressible) Bernoulli equation:

$$\frac{\partial\Phi}{\partial t}+\frac{1}{2}(\nabla\Phi)^2+\int\frac{dP}{\rho}=\text{const or modulo (5)},$$

$$(1-c^2)\frac{\partial\Phi}{\partial t}+\frac{1}{2}v^2=\text{const}.$$

We consider a special situation when the velocity of sound is constant $c^2\approx c_0^2$ (see Refs. 1 and 2).

The above treatment of the potential, nonsteady, compressible flow is not very well known for the class of flows considered. Moreover it goes to the correct equation (see Refs. 1 and 2) without redefinition of the potential as in Thompson's book.[3] Thus all hydronamical quantities $(\mathbf{v},\rho)$ are treated equally in this particular potential approach.

It is easy to notice that the discussed equation (6) is a hyperbolic equation of the second order. We are interested in finding solutions that can be described by means of the Riemann invariant method. According to the requirements of the method we transform Eq. (6) by introducing some new dependent variables into the quasilinear system of equations of the first order,

$$\begin{aligned}&\phi_{0,t}+2(\phi_1\phi_{0,x}+\phi_2\phi_{0,y})+2\phi_1\phi_2\phi_{1,y}+(\phi_1^2-c^2)\phi_{1,x}+(\phi_2^2-c^2)\phi_{2,y}=0,\\&\phi_{0,x}-\phi_{1,t}=0,\quad \phi_{1,y}-\phi_{2,x}=0,\\&\phi_{0,y}-\phi_{2,t}=0,\end{aligned} \tag{7}$$

where we introduce the notation

$$\begin{aligned}&\Phi_{,t}=\phi_0,\quad \Phi_{,x}=\phi_1,\quad \Phi_{,y}=\phi_2,\\&\mathbf{v}=(\phi_1(t,x,y),\phi_2(t,x,y))=\boldsymbol{\phi},\\&\rho=\exp(-\phi_0(t,x,y)).\end{aligned} \tag{8}$$

Thus Eq. (6) is reduced to an undetermined system of four equations for three functions ϕ_0,ϕ_1,ϕ_2.

It is convenient to do the following transformations:

$$t\to t'=c_0t,\quad \phi_0\to\phi_0'=\phi_0/c_0. \tag{9}$$

Then we can write (7) in the following form:

$$\begin{aligned}&\phi_{0,t'}'+2(\phi_1'\phi_{0,x}'+\phi_2'\phi_{0,y}')+2\phi_1'\phi_2'\phi_{1,y}'+(\phi_1'^2-1)\phi_{1,x}'+(\phi_2'^2-1)\phi_{2,y}'=0,\\&\phi_{0,x}'-\phi_{1,t'}'=0,\quad \phi_{1,y}'-\phi_{2,x}'=0,\\&\phi_{0,y}'-\phi_{2,t'}'=0.\end{aligned} \tag{10}$$

The field of velocity of flow $\mathbf{v}$ and the density ρ are in the following form:

$$\mathbf{v}=c_0(\phi_1'(c_0,t,x,y),\phi_2'(c_0t,x,y)),$$

$$\rho=\exp(-c_0\phi_0'(c_0t,x,y)).$$

III. SIMPLE INTEGRAL ELEMENTS

Let us write Eq. (6) using real simple integral elements. We get

$$\gamma^0\lambda_0+2(\phi_1\gamma^0\lambda_1+\phi_2\gamma^0\lambda_2)+2\phi_1\phi_2\gamma^1\lambda_2+(\phi_2^2-c^2)\gamma^2\lambda_2+(\phi_1^2-c^2)\gamma^1\lambda_1=0, \tag{11a}$$

$$\gamma^\mu\lambda_\nu-\gamma^\nu\lambda_\mu=0,\quad \mu,\nu=0,1,2. \tag{11b}$$

From Eq. (11b) we get that the vector γ is proportional to vector λ. Thus, by inserting $\gamma\sim\lambda$ into Eq. (11a) we get a quadratic form with respect to $\lambda_0,\lambda_1,\lambda_2$:

$$Q(\lambda_0,\lambda_1,\lambda_2)=\lambda_0^2+2\lambda_0(\phi_1\lambda_1+\phi_2\lambda_2)+2\phi_1\phi_2\lambda_1\lambda_2+(\phi_1^2-c^2)\lambda_1^2+(\phi_2^2-c^2)\lambda_2^2=0. \tag{12}$$

Now, we follow Ref. 4. We transform the quadratic form (12) to a canonical form. We search for eigenvalues of matrix A (the matrix of the quadratic form Q),

$$\det(A_{ij}-\mu\delta_{ij})=0, \tag{13}$$

where

$$A=\begin{pmatrix}1&\phi_1&\phi_2\\\phi_1&(\phi_1^2-c^2)&\phi_1\phi_2\\\phi_2&\phi_1\phi_2&(\phi_2^1-c^2)\end{pmatrix}.$$

We get the algebraic equation of third order with respect to quantity μ, i.e.,

$$(c^2+\mu)[-\mu^2+\mu(\phi_1^2+\phi_2^2-c^2+1)+c^2]=0.$$

The eigenvalues μ are real,

$$\begin{aligned}&\mu_1=-c^2,\\&\mu_{2,3}=\tfrac{1}{2}(\phi_1^2+\phi_2^2-c^2+1\pm\sqrt{\Delta}),\end{aligned} \tag{14}$$

where $\Delta=(\phi_1^2+\phi_2^2-c^2+1)^2+4c^2>0$. Thus the quadratic form (12) transforms to a canonical form:

$$Q(y,y)=-c^2y_1^2+\tfrac{1}{2}(\phi_1^2+\phi_2^2-c^2+1+\sqrt{\Delta})y_2^2+\tfrac{1}{2}(\phi_1^2+\phi_2^2-c^2+1-\sqrt{\Delta})y_3^2. \tag{15}$$

According to Refs. 4 and 5 we parametrize the convector λ. To do this we search for a parametric equation of (15).

Let us suppose that $y_1\neq0$. Then Eq. (15) may be written in the form

$$\frac{X^2}{a^2}-\frac{y^2}{b^2}=2c^2,\quad \text{where}\quad X=\frac{y_2}{y_1},\quad y=\frac{y_3}{y_1}, \tag{16}$$

and

$$\begin{aligned}&a^2=(\phi_1^2+\phi_2^2-c^2+1+\sqrt{\Delta})^{-1},\\&b^2=(\sqrt{\Delta}-\phi_1^2-\phi_2^2+c^2-1)^{-1}.\end{aligned} \tag{17}$$

If $y_1=0$, $y_2\neq0$, and $y_3\neq0$, then Eq. (15) is as follows:

$$(v^2-c^2+1+\sqrt{\Delta})y_2^2+(v^2-c^2+1-\sqrt{\Delta})y_3^2=0. \tag{18}$$

Equation (16) is the equation of a hyperbola.

Thus we write it in a parametric form

$$X=\sqrt{2}\,ac\cosh\tau,\quad Y=\sqrt{2}\,bc\sinh\tau, \tag{19}$$

where τ is an arbitrary function of ϕ_i, $i=0,1,2$. Thus the covector λ (and consequently γ) became

$$\gamma_1\sim\lambda^1=B\begin{pmatrix}1\\x\\y\end{pmatrix}=B\begin{pmatrix}1\\\sqrt{2}\,ac\cosh\tau\\\sqrt{2}\,bc\sinh\tau\end{pmatrix}, \tag{20}$$

where B is an orthogonal matrix, which diagnolizes the matrix A, i.e.,

$$B^TAB=\begin{pmatrix}\mu_1&0&0\\0&\mu_2&0\\0&0&\mu_3\end{pmatrix},\quad B^T=B^{-1}. \tag{21}$$

Matrix B is built from the eigenvectors of matrix A and takes the form

$$B=h\begin{pmatrix}0&c^2+1-v^2+\sqrt{\Delta}&c^2+1-v^2-\sqrt{\Delta}\\-\phi_2&2\phi_1&2\phi_1\\\phi_1&2\phi_2&2\phi_2\end{pmatrix}, \tag{22}$$

where

$$h=[v^2\{(c^2+1-v^2+\sqrt{\Delta})^2+4v^2\}\times\{(c^2+1-v^2-\sqrt{\Delta})^2+4v^2\}]^{1/2}.$$

Inserting (18) and (22) to (20) we get a covector λ.

In the case with $y_1=0$ we get

$$X=y_3/y_2=\epsilon b/a,\quad \epsilon^2=1. \tag{23}$$

Finally we obtain

$$\gamma_2\sim\lambda^2=B\begin{pmatrix}0\\1\\x\end{pmatrix}=B\begin{pmatrix}0\\1\\\epsilon b/a\end{pmatrix}. \tag{24}$$

Inserting (18) and (22) into (24) we derive a simple element. According to Refs. 4 and 5 we consider the cases with $y_2\neq0$ and after with $y_3\neq0$. We may introduce the following coordinate systems:

$$X=\frac{y_1}{y_2},\quad Y=\frac{y_3}{y_2}\quad\text{or}\quad X=\frac{y_1}{y_3},\quad Y=\frac{y_2}{y_3}.$$

Proceeding as before we get following simple elements:

$$\gamma_3\sim\lambda^3=B\begin{pmatrix}x\\1\\y\end{pmatrix}=B\begin{pmatrix}(1/\sqrt{2}ac)\cos\tau\\1\\(b/a)\sin\tau\end{pmatrix} \tag{25}$$

and

$$\gamma_4\sim\lambda^4=B\begin{pmatrix}x\\y\\1\end{pmatrix}=B\begin{pmatrix}(1/\sqrt{2}bc)\sinh\tau\\(a/b)\cosh\tau\\1\end{pmatrix}. \tag{26}$$

Let us consider cases $y_2=0$ or $y_3=0$. We get

$$X=y_3/y_1=\epsilon bc\sqrt{2}\quad\text{or}\quad X=y_2/y_1=\epsilon ac\sqrt{2}.$$

This time we obtain the following simple elements:

$$\gamma_5\sim\lambda^5=B\begin{pmatrix}1\\0\\x\end{pmatrix}=B\begin{pmatrix}1\\0\\\epsilon bc\sqrt{2}\end{pmatrix} \tag{27}$$

and

$$\gamma_6\sim\lambda^6=B\begin{pmatrix}1\\x\\0\end{pmatrix}=B\begin{pmatrix}1\\\epsilon ac\sqrt{2}\\0\end{pmatrix}. \tag{28}$$

Thus we get here six kinds of simple elements that will be used for construction of solutions, i.e., simple waves and their interactions, the so-called double and multiple waves. All of these simple elements are presented in the Appendix.

IV. SIMPLE WAVES

Now, we present the simplest solutions of Eq. (6), i.e., those which have been constructed on the basis of particular simple integral elements. The method of searching the solutions is presented in Refs. 6–8. According to the terminology used there the elementary solution of a homogeneous system is called a simple wave. These solutions may be regarded as waves since they represent moving disturbances whose profile changes in general in the course of propagation—an indication of this is an implicit form of the relation (4) for function $R(x)$. The form of solution (4) suggests that covector λ should be regarded as an analog of the wave vector $(\omega,\mathbf{k})$ specifying the velocity and direction of a moving wave. A concrete profile of a simple wave is stated explicitly by initial data. However, there exists a certain arbitrariness connected with the freedom of choice of one function of one variable. The above remarks concern all the obtained simple waves. In this paper we apply a method developed in Refs. 4, 5, and 9.

We have the following cases.

A. Case I ($\gamma_1\sim\lambda^1$—see the Appendix)

The simple wave, according to the considerations of Sec. I, is reduced here to fulfilling conditions (3) and (4). Inserting the simple integral element (20) into Eq. (3), we get

$$\frac{d\phi_0}{dR}=c\sqrt{2}\left[\frac{(c^2+1-v^2+\sqrt{\Delta})}{(v^2-c^2+1+\sqrt{\Delta})^{1/2}}\cosh\tau+\frac{(c^2+1-v^2-\sqrt{\Delta})}{(c^2-1-v^2+\sqrt{\Delta})^{1/2}}\sinh\tau\right], \tag{29a}$$

$$\frac{d\phi_1}{dR}=-\phi_2+2c\sqrt{2}\phi_1\left[\frac{\cosh\tau}{(v^2-c^2+1+\sqrt{\Delta})^{1/2}}+\frac{\sinh\tau}{(c^2-1-v^2+\sqrt{\Delta})^{1/2}}\right], \tag{29b}$$

$$\frac{d\phi_2}{dR}=\phi_1+2c\sqrt{2}\phi_2\left[\frac{\cosh\tau}{(v^2-c^2+1+\sqrt{\Delta})^{1/2}}+\frac{\sinh\tau}{(c^2-1-v^2+\sqrt{\Delta})^{1/2}}\right], \tag{29c}$$

where $v^2=\phi_1^2+\phi_2^2$, $\Delta=(v^2-c^2+1)^2+4c^2$. We are interested here in solving the system (7) with respect to the potential of the velocity field $\mathbf{v}=(\phi_1,\phi_2)$ and density $\rho=\exp(-\phi_0)$. Now, let us assume that the expression in the square brackets in Eqs. (29b) and (29c) is a smooth function of v^2, i.e.,

$$\frac{\cosh\tau}{(v^2-c^2+1+\sqrt{\Delta})^{1/2}}+\frac{\sinh\tau}{(c^2-1-v^2+\sqrt{\Delta})^{1/2}}=f(v^2). \tag{30}$$

That means $\tau=\tau(v^2)=\tau(R)$.

In this case we are able to find a solution in a closed form. We introduce the quantity $\mu_0=\phi_1/\phi_2$. Now we divide Eq. (29b) [resp. Eq. (29c)] by ϕ_1 (resp. ϕ_2). Then we subtract both sides and finally we integrate and obtain

$$\mu_0=\tan(c_1-R),\quad c_1=\text{const.} \tag{31}$$

Then we introduce the quantity $v^2=\phi_1^2+\phi_2^2$. Thus, by multiplying Eq. (29b) by ϕ_1 and (29c) and ϕ_2 and summing both sides, and then integrating we have

$$F(v^2)=\int_a^{v^2}\frac{dr}{crf(r)}=8\sqrt{2}R+c_2, \tag{32}$$

where a, $c_2=\text{const}$.

Now we assume there exists an inverse function G of F, such that

$$G(F(r))=r,\quad r>0,$$

and we get

$$v^2=G(s),\quad \text{where } s=8\sqrt{2}R+c_2. \tag{33}$$

Function G is an arbitrary non-negative function and it obeys the equation

$$\frac{dG}{ds}=\left(\frac{dF}{dv^2}\right)^{-1}=f(G(s)). \tag{34}$$

From equations (31) and (33) we can calculate

$$\begin{aligned}\phi_1&=\epsilon G^{1/2}(8\sqrt{2}R+c_2)\sin(c_1-R),\\ \phi_2&=\epsilon G^{1/2}(8\sqrt{2}R+c_2)\cos(c_1-R),\quad \epsilon^2=1.\end{aligned} \tag{35}$$

Inserting (35) into (30) and simultaneously using relations (32) and (34) and then introducing $G=e^{2H}$ we obtain

$$\left.\frac{dH}{ds}\right|_{s=8\sqrt{2}R+c_2}=\frac{1}{2c}\left[\frac{\cosh\tau}{(1+e^{2H}-c^2+\sqrt{\Delta})^{1/2}}+\frac{\sinh\tau}{(c^2-1-e^{2H}+\sqrt{\Delta})^{1/2}}\right], \tag{36}$$

$$\Delta=(e^{2H}-c^2+1)^2+4c^2,$$

where H is an arbitrary function of s. So, it is obvious that if function τ is given, then function H is given as well, and vice versa. But function H is more convenient for parametrizing the simple element. Since we regard the quantity τ as given, we are led to solve an ordinary differential equation with respect to H. Thus, from Eq. (36) we get

$$e^{\tau}=\alpha/2\sqrt{\Delta},$$

where

$$\alpha=4\frac{dH}{ds}+2\left(8\left(\frac{dH}{ds}\right)^2+e^{2H}+1-c^2\right)^{1/2} \tag{37}$$

and

$$\cosh\tau=\frac{\alpha^2+4\Delta}{4\alpha\sqrt{\Delta}},\quad \sinh\tau=\frac{\alpha^2-4\Delta}{4\alpha\sqrt{\Delta}}. \tag{38}$$

As in Ref. 5 we search for a restriction of the function H. It is obvious that it must be

$$\begin{aligned}&(1)\quad 8\left(\frac{dH}{ds}\right)^2+e^{2H}+1-c^2\geqslant 0,\\ &(2)\quad \alpha>0.\end{aligned} \tag{39}$$

Condition (2) is easily satisfied by assuming that $dH/ds\geqslant 0$. If $c=\text{const}$, we may substitute $c=1$ and both conditions are always satisfied [cf. Sec. II, Eqs. (9) and (10)]. Hence, the simple wave corresponding to the simple element (22) has the form

$$\begin{aligned}&\mathbf{v}=\epsilon\exp[H(8\sqrt{2}R+c_2)](\sin(c_1-R),\cos(c_1-R)),\\ &\epsilon^2=1.\end{aligned} \tag{40}$$

Function $R=R(t,x,y)$ is understood according to the expression (4) which means that the three-dimensional vector $\nabla R(t,x,y)$ is proportional to vector λ [1]. Then

$$\begin{aligned}R=\Psi\Bigg(&\frac{\sqrt{2}c}{4\alpha\sqrt{\Delta}}\left[\frac{2-e^{2H}+\sqrt{\Delta}}{(e^{2H}+\sqrt{\Delta})^{1/2}}(\alpha^2+4\Delta)+\frac{2-e^{2H}-\sqrt{\Delta}}{(-e^{2H}+\sqrt{\Delta})^{1/2}}(\alpha^2-4\Delta)\right]t\\ &+\epsilon\exp H\left\{\left[4\sqrt{2}\frac{dH}{ds}\sin(c_1-R)-\cos(c_1-R)\right]x+4\sqrt{2}\left[\frac{dH}{ds}\cos(c_1-R)+\sin(c_1-R)\right]y\right\}\Bigg).\end{aligned} \tag{41}$$

The density ρ is given by

$$\rho=\rho_0\exp(-\phi_0),\quad \rho_0=\text{const}, \tag{42}$$

where ϕ_0 is the following:

$$\begin{aligned}\phi_0=\int_{R_0}^{R}&\frac{c\,dR'}{\sqrt{2}(4\,dH/ds+[2(8(dH/ds)^2+e^{2H}-1-c^2)]^{1/2})((e^{2H}-c^2+1)^2+4c^2)^{1/2}}\\ &\times\Bigg\{\frac{c^2+1-e^{2H}+((e^{2H}-c^2+1)^2+4c^2)^{1/2}}{[e^{2H}-c^2+1+((e^{2H}-c^2+1)^2+4c^2)]^{1/2}}\left(16\left(\frac{dH}{ds}\right)^2+4\frac{dH}{ds}\left[2\left(8\left(\frac{dH}{ds}\right)^2+e^{2H}-1-c^2\right)\right]^{1/2}\right.\\ &\left.+2e^{4H}+2c^4+1-4c^2e^{2H}+5e^{2H}+8c^2\right)+\frac{c^2-1-e^{2H}-((e^{2H}-c^2+1)^2+4c^2)^{1/2}}{[c^2-1-e^{2H}+((e^{2H}-c^2+1)^2+4c^2)^{1/2}]}\\ &\times\left(16\left(\frac{dH}{ds}\right)^2+4\frac{dH}{ds}\left[2\left(8\left(\frac{dH}{ds}\right)^2+e^{2H}-1-c^2\right)\right]^{1/2}-2e^{4H}-2c^4-3+4c^2e^{2H}-3e^{2H}-5c^2\right)\Bigg\}.\end{aligned} \tag{43}$$

Function H is a function of $s = 8\sqrt{2}R + c_2$ and is arbitrary ($c = \text{const}$) and $dH/ds > 0$.

Now we introduce the quantity

$$\delta = \lambda_0 + \mathbf{v} \cdot \boldsymbol{\lambda}, \tag{44}$$

which has a physical interpretation as a velocity of a moving wave with respect to the medium, whereas λ_0 is a local velocity of the wave. In our case δ and λ_0 take the following form:

$$\lambda_0 = \frac{\sqrt{2}}{4\alpha\sqrt{\Delta}}\left[\frac{c^2 - e^{2H} + \sqrt{\Delta}}{(e^{2H} + \sqrt{\Delta})^{1/2}}(\alpha^2 + 4\Delta) + \frac{2 - e^{2H} - \sqrt{\Delta}}{(-e^{2H} + \sqrt{\Delta})^{1/2}}(\alpha^2 - 4\Delta)\right],$$

$$\delta = \lambda_0 + \exp(2H)\left\{\left[4\sqrt{2}\frac{dH}{ds}\sin(c_1 - R) - \cos(c_1 - R)\right]\sin(c_1 - R)\right.$$

$$\left. + \left[4\sqrt{2}\frac{dH}{ds}\cos(c_1 - R) + \sin(c_1 - R)\right]\cos(c_1 - R)\right\}. \tag{45}$$

B. Case II ($\gamma_2 \sim \lambda^2$—see the Appendix)

A simple wave corresponding to the simple integral element (24) may be found by integrating the following system of equations:

$$\frac{d\phi_0'}{dR} = (2 - v^2 + \sqrt{\Delta})(\sqrt{\Delta} - v^2)^{1/2} + (2 - v^2 - \sqrt{\Delta})(v^2 + \sqrt{\Delta})^{1/2}, \tag{46a}$$

$$\frac{d\phi_1'}{dR} = 2\phi_1'[2(\sqrt{\Delta} + 2)]^{1/2}, \tag{46b}$$

$$\frac{d\phi_2'}{dR} = 2\phi_2'[2(\sqrt{\Delta} + 2)]^{1/2}, \tag{46c}$$

where $v^2 = \phi_1'^2 + \phi_2'^2$, $\Delta = v^4 + 4$. We assume here that the velocity of sound $c = 1$. By dividing both sides of Eqs. (29b) and (29c) and the integrating we get

$$\phi_1' = c_1\phi_2', \quad c_1 = \text{const}. \tag{47}$$

Now, we calculate the quantity v:

$$v = [(1/(c_2 - 2\sqrt{2}R)^2 - 2)^2 - 4]^{1/4}, \quad c_2 = \text{const}. \tag{48}$$

Hence we obtain

$$\phi_1' = \frac{\epsilon c_1}{\sqrt{c_1^2 + 1}}\left[\left(\frac{1}{(c_2 - 2\sqrt{2}R)^2} - 2\right)^2 - 4\right]^{1/4}, \quad \phi_2' = \frac{\epsilon}{\sqrt{c_1^2 + 1}}\left[\left(\frac{1}{(c_2 - 2\sqrt{2}R)^2} - 2\right)^2 - 4\right]^{1/4}, \quad \epsilon^2 = 1. \tag{49}$$

Substituting (48) into (29a) and then integrating, we have

$$\phi_0' = -6\left[\sqrt{2}(c_2 - 2\sqrt{2}R) + \arctan\frac{1 - (1 - 2(c_2 - 2\sqrt{2}R)^2)^{1/2}}{\sqrt{2}(c_2 - 2\sqrt{2}R)}\right]. \tag{50}$$

Thus a simple wave corresponding to the simple (24) has the following form:

$$\mathbf{v} = \frac{\epsilon c}{\sqrt{c_1^2 + 1}}\left[\left(\frac{1}{(c_2 - 2\sqrt{2}R)^2} - 2\right)^2 - 4\right]^{1/4}(c_1, 1),$$

$$\rho = \rho_0 \exp\left[6c\sqrt{2}(c_2 - 2\sqrt{2}R) + \arctan\frac{1 - (1 - 2(c_2 - 2\sqrt{2}R)^2)^{1/2}}{\sqrt{2}(c_2 - 2\sqrt{2}R)}\right]. \tag{51}$$

The dependent variable R, i.e., the Riemann invariant, is given explicitly by the formula

$$R = \Psi\left(\left[\left(\frac{1}{(c_2 - 2\sqrt{2}R)^2} - \left[\left(\frac{1}{(c_2 - 2\sqrt{2}R)^2} - 2\right)^2 - 4\right]^{1/2}\right)\left(\frac{1}{(c_2 - 2\sqrt{2}R)^2} - 2 - \left[\left(\frac{1}{(c_2 - 2\sqrt{2}R)^2} - 2\right)^2 - 4\right]^{1/2}\right)^{1/2}\right.$$

$$+ \left(4 - \left[\left(\frac{1}{(c_2 - 2\sqrt{2}R)^2} - 2\right)^2 - 4\right]^{1/2} - \frac{1}{(c_2 - 2\sqrt{2}R)^2}\right)\left(\left[\left(\frac{1}{(c_2 - 2\sqrt{2}R)^2} - 2\right)^2 - 4\right]^{1/2}\right.$$

$$\left.\left. + \frac{1}{(c_2 - 2\sqrt{2}R)^2} - 2\right)^{1/2}\right]ct + \frac{2\epsilon}{(c_1^2 + 1)^{1/2}}\left[\left(\frac{1}{(c_2 - 2\sqrt{2}R)^2} - 2\right)^2 - 4\right]^{1/4}$$

$$\times\left\{\left(\frac{1}{(c_2 - 2\sqrt{2}R)^2} - 2 - \left[\left(\frac{1}{(c_2 - 2\sqrt{2}R)^2} - 2\right)^2 - 4\right]^{1/2}\right)^{1/2}\right.$$

$$\left. + \left(\frac{1}{(c_2 - 2\sqrt{2}R)^2} - 2 + \left[\left(\frac{1}{(c_2 - 2\sqrt{2}R)^2} - 2\right)^2 - 4\right]^{1/2}\right)^{1/2}\right\}(c_1 x + y)\Bigg), \tag{52}$$

where Ψ is an arbitrary function of one variable. The solution (51) with condition (52) describes one-dimensional, nonstationary flow that goes in the direction $(c_1, 1)$. It is worth mentioning that the solution is defined everywhere except $R_0 = c_2/2\sqrt{2}$. The quantities λ_0 and δ (the total velocity of the wave and the velocity of the wave with respect to the medium) are as follows:

$$\lambda_0 = c\left[\left(\frac{1}{(c_2-2\sqrt{2}R)^2}-\left[\left(\frac{1}{(c_2-2\sqrt{2}R)^2}-2\right)^2-4\right]^{1/2}\right)\left(\frac{1}{(c_2-2\sqrt{2}R)^2}-2-\left[\left(\frac{1}{(c_2-2\sqrt{2}R)^2}-2\right)^2-4\right]^{1/2}\right)^{1/2}\right.$$
$$\left.+\left(4-\left[\left(\frac{1}{(c_2-2\sqrt{2}R)^2}-2\right)^2-4\right]^{1/2}-\frac{1}{(c_2-2\sqrt{2}R)^2}\right)\left(\left[\left(\frac{1}{(c_2-2\sqrt{2}R)^2}-2\right)^2-4\right]^{1/2}+\frac{1}{(c_2-2\sqrt{2}R)^2}-2\right)\right], \tag{53}$$

$$\delta = \lambda_0 + 2\epsilon(c_1^2+1)^{1/2}\left[\left(\frac{1}{(c_2-2\sqrt{2}R)^2}-2\right)^2-4\right]^{1/2}\left\{\left(\frac{1}{(c_2-2\sqrt{2}R)^2}-2-\left[\left(\frac{1}{(c_2-2\sqrt{2}R)^2}-2\right)^2-4\right]^{1/2}\right)^{1/2}\right.$$
$$\left.+\left(\frac{1}{(c_2-2\sqrt{2}R)^2}-2+\left[\left(\frac{1}{(c_2-2\sqrt{2}R)^2}-2\right)^2-4\right]^{1/2}\right)^{1/2}\right\}.$$

Moreover we have a restriction:

$$(1/(c_2-2\sqrt{2}R)^2-2)^2-4\geqslant 0. \tag{54}$$

This inequality may be easily solved and we obtain

$$R\geqslant (c_2-2)/2\sqrt{2} \quad \text{or} \quad R\leqslant (2+c_2)/2\sqrt{2}.$$

C. Case III ($\gamma_3 \sim \lambda^3$—see the Appendix)

A simple wave corresponding to simple integral elements (25) may be found by integrating the following system of ordinary differential equations:

$$\frac{d\phi_0}{dR} = (c^2+1-v^2+\sqrt{\Delta})+(c^2+1-v^2-\sqrt{\Delta})\times\frac{(v^2-c^2+1+\sqrt{\Delta})^{1/2}}{(c^2-1-v^2+\sqrt{\Delta})^{1/2}}\sin\tau,$$
$$\frac{d\phi_1}{dR} = \frac{-\phi_2}{c\sqrt{2}}(v^2-c^2+1+\sqrt{\Delta})^{1/2}\cos\tau + 2\phi_1\left[1+\left(\frac{v^2-c^2+1+\sqrt{\Delta}}{c^2-1-v^2+\sqrt{\Delta}}\right)^{1/2}\sin\tau\right], \tag{55}$$
$$\frac{d\phi_2}{dR} = \frac{\phi_1}{c\sqrt{2}}(v^2-c^2+1+\sqrt{\Delta})^{1/2}\cos\tau + 2\phi_2\left[1+\left(\frac{v^2-c^2+1+\sqrt{\Delta}}{c^2-1-v^2-\sqrt{\Delta}}\right)^{1/2}\sin\tau\right],$$

where $v^2=\phi_1^2+\phi_2^2$, $\Delta=(v^2-c^2+1)^2+4c^2$.

To solve the equations it is convenient to introduce a new variable $\mu_0=\phi_1/\phi_2$. For quantities μ_0 and v^2 we obtain the following system of equations:

$$\frac{dv^2}{dR} = \left[1+\left(\frac{v^2-c^2+1+\sqrt{\Delta}}{c^2-1-v^2+\sqrt{\Delta}}\right)^{1/2}\sin\tau\right], \tag{56}$$

$$\frac{d}{dR}\arctan\mu_0 = \frac{(\sqrt{\Delta}-v^2+c^2-1)^{1/2}}{c\sqrt{2}}\cos\tau, \tag{57}$$

where τ is an arbitrary function of R. It is convenient to substitute

$$v^2 = e^{2H} \tag{58}$$

and H parametrizes the simple element (25).

We find the restrictions for H. Substituting (58) into (56) we have

$$\frac{1}{2}\left|\left(\frac{dH}{dR}-2\right)\left(\frac{c^2-1-e^{2H}+\sqrt{\Delta}}{e^{2H}-c^2+1+\sqrt{\Delta}}\right)\right| = |\sin\tau|\leqslant 1. \tag{59}$$

Using the relations between trigonometrical functions we calculate $\cos\tau$ and substitute into (57)

$$\frac{d}{dR}\arctan\mu_0 = \epsilon_1\frac{(\sqrt{\Delta}-e^{2H}+c^2-1)^{1/2}}{c\sqrt{2}}\times\left[+-\frac{1}{4}\left(\frac{dH}{dR}-2\right)^2\frac{(c^2-1-e^{2H}+\sqrt{\Delta})}{(e^{2H}-c^2+1+\sqrt{\Delta})}\right]^{1/2},$$
$$\epsilon_1^2=1. \tag{60}$$

The differential inequality (59) leads us to the solution for which the length of vector $\mathbf{v}$ is constant, i.e., $H=H_0=\text{const}$. Then by inserting quantity $H=H_0$ into (56) and (57) and integrating we get finally

$$\mathbf{v} = ce^{H_0}(\epsilon_2\sin(K(R)+c_1),\cos(K(R)+c_1)),$$
$$\rho = \rho_0\exp[-2c(R-R_0)(2-e^{2H_0})],$$
$$K(R) = \epsilon_1\left[\frac{e^{2H_0}[(e^{4H_0}+4)^{1/2}-e^{2H_0}]}{(e^{4H_0}+4)^{1/2}+e^{2H_0}}\right](R-R_0),$$
$$\epsilon_1^2=\epsilon_2^2=1, \tag{61}$$
$$R = \Psi(2c(2-e^{2H_0})t+e^{H_0}\{[4\epsilon_2\sin(K(R)+c_1) - \epsilon_1 e^{H_0}\cos(K(R)+c_1)]x + [4\cos(K(R)+c_1)+\epsilon_1\epsilon_2 e^{H_0}\sin(K(R)+c_1)]y\}).$$

Quantities λ_0 and δ_0 are

$$\lambda_0 = 2c(2-2^{eH_0}),$$
$$\delta = 2c(2-e^{2H_0})+4e^{2H_0}, \tag{62}$$

and c is the velocity of sound.

D. Case IV ($\gamma_5 \sim \lambda^5$—see the Appendix)

A simple wave corresponding to simple integral element (27) may be found by integrating the following system of

ordinary differential equations:

$$\frac{d\phi_0'}{dR} = \frac{\epsilon_1\sqrt{2}(2 - v^2 + \sqrt{\Delta})}{(\sqrt{\Delta} - v^2)^{1/2}}, \tag{63a}$$

$$\frac{d\phi_1'}{dR} = -\phi_2' + 2\phi_1' \frac{\epsilon_1\sqrt{2}}{(\sqrt{\Delta} - v^2)^{1/2}}, \tag{63b}$$

$$\frac{d\phi_2'}{dR} = -\phi_1' + 2\phi_2' \frac{\epsilon_1\sqrt{2}}{(\sqrt{\Delta} - v^2)^{1/2}}, \tag{63c}$$

where $\Delta = v^4 + 4$, $v^2 = \phi_1'^2 + \phi_2'^2$, and we have assumed that the velocity of sound equals 1. By dividing Eq. (63b) by ϕ_1' and Eq. (63c) by ϕ_2' and subtracting both sides of them and integrating, we obtain

$$\phi_1'/\phi_2' = \tan(c_1 - R), \quad c_1 = \text{const.} \tag{64}$$

Then we calculate v^2. We get

$$F(v^2) = \tfrac{2}{3}((v^4 + 4)^{1/2} - v^2)^{3/2} + 4\sqrt{2}\arctan\left(\frac{(v^4 + 4)^{1/2} - v^2}{2}\right)^{1/2} + 2\sqrt{2}\ln\frac{((v^4 + 4)^{1/2} - v^2)^{1/2} - \sqrt{2}}{((v^4 + 4)^{1/2} - v^2)^{1/2} - \sqrt{2}} = 4\sqrt{2}R + c_2,$$

$$c_2 = \text{const.} \tag{65}$$

Function F is monotone and consequently it has an inverse function G. Thus we have

$$v^2 = G(4\sqrt{2}R + c_2). \tag{66}$$

The domain of G is $(-\infty, +\infty)$ and its range is $(0, +\infty)$.

From equations (64), (66), and (63a) we get

$$\begin{aligned}
\phi_1' &= \epsilon_2 G^{1/2}(4\sqrt{2}R + c_2)\sin(c_1 - R), \\
\phi_2' &= \epsilon_2 G^{1/2}(4\sqrt{2}R + c_2)\cos(c_1 - R), \\
\phi_0' &= \epsilon_2\sqrt{2}\int_{R_0}^{R} \frac{(2 - G + (G^2 + 4)^{1/2})}{((G^2 + 4)^{1/2} - G)^{1/2}}\, dR' + c_3, \\
c_3 &= \text{const},
\end{aligned} \tag{67}$$

where $G(F(x)) = x$ and G is a function of $4\sqrt{2}R + c_2$.

Thus the simple wave corresponding to the simple element (27) is

$$\mathbf{v} = \epsilon_2 c G^{1/2}(4\sqrt{2}R + c_2)(\sin(c_1 - R), \cos(c_1 - R)), \tag{68}$$

$$\rho = \rho_0 \exp\left(-\epsilon_2 c\sqrt{2}\int_{R_0}^{R} \frac{(2 - G + (G^2 + 4)^{1/2})}{((G^2 + 4)^{1/2} - G)^{1/2}}\, dR'\right).$$

The dependent variable R (i.e., Riemann invariant) is given in an implicit form

$$R = \Psi\left(\left[\frac{\epsilon_1\sqrt{2}(2 - G + (G^2 + 4)^{1/2})}{((G^2 + 4)^{1/2} - G)^{1/2}}\right] ct + \epsilon_2 G^{1/2}\left\{\left[2\sin(c_1 - R)\frac{\epsilon_1\sqrt{2}}{((G^2 + 4)^{1/2} - G)^{1/2}} - \cos(c_1 - R)\right]x + \left[2\cos(c_1 - R)\frac{\epsilon_1\sqrt{2}}{((G^2 + 4)^{1/2} - G)^{1/2}} + \sin(c_1 - R)\right]y\right\}\right), \tag{69}$$

where Ψ is an arbitrary function of one variable. The quantities λ_0, δ, i.e., respectively a local wave velocity and velocity of a moving wave with respect to the medium, equal

$$\lambda_0 = \frac{c\epsilon_1\sqrt{2}(2 - G + (G^2 + 4)^{1/2})}{((G^2 + 4)^{1/2} - G)^{1/2}}, \quad \delta = \frac{\epsilon_1\sqrt{2}(2 + G + (G^2 + 4)^{1/2})}{((G^2 + 4)^{1/2} - G)^{1/2}}. \tag{70}$$

E. Case V ($\gamma_4 \sim \lambda^4$—see the Appendix)

A simple wave corresponding a simple element (26) can be found by integration of the following system of equations:

$$\begin{aligned}
\frac{d\phi_0}{dR} &= (c^2 + 1 - v^2 - \sqrt{\Delta})\left(\frac{\sqrt{\Delta} + v^2 + c^2 - 1}{\sqrt{\Delta} + v^2 - c^2 + 1}\right)^{1/2}\cosh\tau + (c^2 + 1 - v^2 - \sqrt{\Delta}), \\
\frac{d\phi_1}{dR} &= \frac{-\phi_2}{c\sqrt{2}}(\sqrt{\Delta} - v^2 + c^2 - 1)^{1/2}\sinh\tau + 2\phi_1\left[1 + \left(\frac{1\sqrt{\Delta} - v^2 + c^2 - 1}{\sqrt{\Delta} + v^2 - c^2 + 1}\right)^{1/2}\cosh\tau\right], \\
\frac{d\phi_2}{dR} &= \frac{\phi_1}{c\sqrt{2}}(\sqrt{\Delta} - v^2 + c^2 - 1)^{1/2}\sinh\tau + 2\phi_2\left[1 + \left(\frac{\sqrt{\Delta} - v^2 + c^2 - 1}{\sqrt{\Delta} + v^2 - c^2 + 1}\right)^{1/2}\cosh\tau\right],
\end{aligned} \tag{71}$$

where $v^2 = \phi_1^2 + \phi_2^2$, $\Delta = (v^2 - c^2 + 1)^2 + 4c^2$.

We introduce new dependent variables v^2 and $\mu_0 = \phi_1/\phi_2$ and we get

$$\frac{1}{2}\frac{dv^2}{dR} = 2v^2\left[1 + \left(\frac{v^2 - c^2 + 1 + \sqrt{\Delta}}{c^2 - 1 - v^2 + \sqrt{\Delta}}\right)^{1/2}\cosh\tau\right], \tag{72}$$

$$\frac{d}{dR}\arctan\mu_0 = \frac{(\sqrt{\Delta} - v^2 + c^2 - 1)^{1/2}}{c\sqrt{2}}\sinh\tau, \tag{73}$$

where τ is an arbitrary function of R. It is convenient to substitute

$$v^2 = e^{2H}. \tag{74}$$

Thus, the simple element (26) may be parametrized by function H instead of τ and we find restriction for H. By inserting (74) into (72) we find

$$1 \leqslant \cosh\tau = \frac{1}{2}\left(\frac{dH}{dR} - 1\right)\left(\frac{c^2 - 1 - e^{2H} + \sqrt{\Delta}}{e^{2H} - c^2 + 1 + \sqrt{\Delta}}\right)^{1/2}. \tag{75}$$

Using relations between hyperbolic functions we calculate the quantity $\sinh\tau$ and then substitute it into Eq. (73) to get

$$\frac{d}{dR}\arctan\mu_0 = \frac{\epsilon_1(\sqrt{\Delta} - e^{2H} + c^2 - 1)^{1/2}}{c\sqrt{2}}\left[1 - \frac{1}{4}\left(\frac{dH}{dR} - 2\right)^2 \frac{(\sqrt{\Delta} - e^{2H} + c^2 + 1)}{(\sqrt{\Delta} + e^{2H} - c^2 + 1)}\right]^{1/2}, \quad \epsilon_1^2 = 1. \tag{76}$$

The differential inequality (75) leads to a solution for which the function H is constant, $H = H_0 = \text{const}$. It means that the length of the vector $\mathbf{v}$ is constant. Thus by substituting $H = H_0$ into Eqs. (71) and (76) and then integrating, we get

$$\begin{aligned} &\phi_1' = \epsilon_2 e^{H_0}\sin(K(R) + c_1), \quad \epsilon_2^2 = 1, \\ &\phi_2' = e^{H_0}\cos(K(R) + c_1), \end{aligned} \tag{77}$$

where

$$K(R) = \epsilon_1\left[\frac{e^{2H_0}(\sqrt{\Delta} - e^{2H_0} + 2)}{(\sqrt{\Delta} + e^{2H_0})}\right]^{1/2}(R - R_0), \quad \Delta = e^{4H_0} + 4, \quad c_1 = \text{const},$$

and

$$\phi_0' = c_2 + \left[-(2 - e^{2H_0} + \sqrt{\Delta})(\sqrt{\Delta} - e^{2H_0})/(\sqrt{\Delta} + e^{2H_0}) + (2 - e^{2H_0} - \sqrt{\Delta})\right](R - R_0), \tag{78}$$

where $c_2 = \text{const}$.

Finally, we have

$$\begin{aligned} &\mathbf{v} = c\, e^{H_0}(\epsilon_2\sin(K(R) + c_1), \cos(K(R) + c_1)), \\ &\rho = \rho_0\exp\left\{c\left[(2 - e^{2H_0} + \sqrt{\Delta})(\sqrt{\Delta} - e^{2H_0})/(\sqrt{\Delta} + e^{2H_0}) - (2 - e^{2H_0} - \sqrt{\Delta})\right](R - R_0)\right\}, \quad \rho_0 = \text{const}. \end{aligned} \tag{79}$$

The Riemann invariant R is given in an implicit form as

$$\begin{aligned} R = \Psi\Bigg(&\left[(2 - e^{2H_0} - \sqrt{\Delta}) - (2 - e^{2H_0} + \sqrt{\Delta})\frac{\sqrt{\Delta} - e^{2H_0}}{\sqrt{\Delta} + e^{2H_0}}\right]ct \\ &+ e^{H_0}\Bigg\{\left[4\epsilon_2\frac{e^{2H_0}}{\sqrt{\Delta} + e^{2H_0}}\sin(K(R) + c_1) - \frac{\epsilon_1(\sqrt{\Delta} - e^{2H_0})^{1/2}e^{H_0}}{(\sqrt{\Delta} + e^{2H_0})^{1/2}}\cos(K(R) + c_1)\right]x \\ &+ \left[4\frac{e^{2H_0}}{\sqrt{\Delta} + e^{2H_0}}\cos(K(R) + c_1) + \frac{\epsilon_1\epsilon_2(\sqrt{\Delta} - e^{2H_0})^{1/2}}{(\sqrt{\Delta} + e^{2H_0})^{1/2}}\sin(K(R) + c_1)\right]y\Bigg\}\Bigg), \end{aligned} \tag{80}$$

where Ψ is an arbitrary function of one variable. A local wave velocity and velocity of wave with respect to the medium are constant and given by

$$\lambda_0 = c\left[(2 - e^{2H_0} - \sqrt{\Delta}) - (2 - e^{2H_0} + \sqrt{\Delta})\frac{(\sqrt{\Delta} - e^{2H_0})}{(\sqrt{\Delta} + e^{2H_0})}\right], \quad \delta = \lambda_0 + \frac{4e^{4H_0}}{\sqrt{\Delta} + e^{2H_0}}, \tag{81}$$

where $c = \text{const}$ and it is the velocity of sound.

F. Case VI ($\gamma_6 \sim \lambda^6$—see the Appendix)

A simple wave corresponding to the simple element (28) may be found by integration of following system of equations:

$$\begin{aligned} &\frac{d\phi_0'}{dR} = \frac{\epsilon_1\sqrt{2}(2 - v^2 + \sqrt{\Delta})}{(v^2 + \sqrt{\Delta})^{1/2}}, \quad \epsilon_1^2 = 1, \\ &\frac{d\phi_1'}{dR} = -\phi_2' + 2\phi_1'\frac{\epsilon_1\sqrt{2}}{(v^2 + \sqrt{\Delta})^{1/2}}, \\ &\frac{d\phi_2'}{dR} = \phi_1' + 2\phi_2'\frac{\epsilon_1\sqrt{2}}{(v^2 + \sqrt{\Delta})^{1/2}}, \end{aligned} \tag{82}$$

where $\Delta = v^4 + 4$, $v^2 = \phi_1'^2 + \phi_2'^2$.

We assume that the velocity of sound equals 1. We introduce new variables $\mu_0 = \phi_1'/\phi_2'$ and v^2.

As before we integrate equations for these variables and we get

$$\mu_0 = \phi_1'/\phi_2' = \tan(c_1 - R), \quad c_1 = \text{const}, \tag{83}$$

$$F_1(v^2) = -2\arctan\left(\frac{(v^4+4)^{1/2}-v^2}{2}\right)^{1/2} + (2((v^4+4)^{1/2}-v^2))^{1/2}$$

$$+ \ln\left[\frac{((v^4+4)^{1/2}-v^2)^{1/2}-\sqrt{2}}{((v^4+4)^{1/2}-v^2)^{1/2}+\sqrt{2}}\right] = 2\epsilon_1\sqrt{2}R + c_2, \quad c_2 = \text{const}. \tag{84}$$

Function F_1 is monotone. So, in the interval $(0, +\infty)$ it possesses an inverse function G_1 such as

$$G_1(F_1(x)) = x. \tag{85}$$

We get

$$v^2 = G_1(2\epsilon_1\sqrt{2}R + c_2).$$

From (83), (85), and (82) we have

$$\begin{aligned}
\phi_1' &= \epsilon_2 G_1^{1/2}(2\epsilon_1\sqrt{2}R + c_1)\sin(c_1 - R),\\
\phi_2' &= \epsilon_2 G^{1/2}(2\epsilon_1\sqrt{2}R + c_1)\cos(c_1 - R),\\
\phi_0' &= \epsilon_1\sqrt{2}\int_{R_0}^{R} \frac{(2 - G + (G^2+4)^{1/2})}{((G^2+4)^{1/2}+G)^{1/2}}\,dR' + c_3, \quad c_3 = \text{const},
\end{aligned} \tag{86}$$

where the function G_1 is given by a transcendent equation

$$(2((c_1^2+4)^{1/2}-G))^{1/2} + \ln\left[\frac{((G_1^2+4)^{1/2}-G_1)^{1/2}-\sqrt{2}}{((G_1^2+4)^{1/2}-G_1)^{1/2}+\sqrt{2}}\right] - 2\arctan\left(\frac{(G_1^2+4)^{1/2}-G_1}{2}\right)^{1/2} = 2\epsilon_1\sqrt{2}R + c_2. \tag{87}$$

Thus a simple wave corresponding to the simple element (28) is

$$\begin{aligned}
\mathbf{v} &= \epsilon_2 G_1^{1/2}(2\epsilon_1\sqrt{2}R + c_2)(\sin(c_1 - R), \cos(c_1 - R)),\\
\rho &= \rho_0 \exp\left(-c\epsilon_1\sqrt{2}\int_{R_0}^{R} \frac{(2 - G_1 + (G_1^2+4)^{1/2})}{((G_1^2+4)^{1/2}+G_1)^{1/2}}\,dR'\right).
\end{aligned} \tag{88}$$

The dependent variable R, the Riemann invariant, is given in implicit form as

$$R = \Psi\left(\left[\frac{\epsilon_1\sqrt{2}(2 - G + (G^2+4)^{1/2})}{(G + (G^2+4)^{1/2})^{1/2}}\right]ct + \epsilon_2 G^{1/2}\left\{\left[\frac{2\epsilon_1\sqrt{2}}{(G + (G^2+4)^{1/2})^{1/2}}\sin(c_1 - R) - \cos(c_1 - R)\right]x\right.\right.$$

$$\left.\left. + \left[\frac{2\epsilon_1\sqrt{2}}{(G + (G^2+4)^{1/2})^{1/2}}\cos(c_1 - R) + \sin(c_1 - R)\right]y\right\}\right), \tag{89}$$

where Ψ is an arbitrary function of one variable.

Quantities λ_0, δ, which are, respectively, the local wave velocity and the velocity of wave with respect to the medium, are given by

$$\lambda_0 = \frac{c\epsilon_1\sqrt{2}(2 - G_1 + (G_1^2+4)^{1/2})}{(c_1 + (G_1^2+4)^{1/2})^{1/2}}, \quad \delta = \frac{\epsilon_1\sqrt{2}(2 + G_1 + (G_1^2+4)^{1/2})}{(G_1 + (G_1^2+4)^{1/2})^{1/2}}. \tag{90}$$

The above-described simple waves are the basis for searching for a wider class of solution, the so-called double waves and multiple waves. The superpositions of this type may be very interesting from the physical point of view and they will be considered in future papers.

It is interesting to notice that our calculations can be extended to the three-dimensional case. However, it will cause very tedious and laborious algebra. It seems that the assumption of the constancy of the velocity of sound can be abandoned. However, we cannot use some mathematical tricks in the above calculations and probably we cannot get compact results.

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APPENDIX: SIMPLE ELEMENTS

The covectors λ are

$$\lambda^1=\begin{pmatrix} c\sqrt{2}\left[\dfrac{(c^2+1-v^2+\sqrt{\Delta})}{(v^2-c^2+1+\sqrt{\Delta})^{1/2}}\cosh\tau+\dfrac{(c^2+1-v^2-\sqrt{\Delta})}{(c^2-1-v^2+\sqrt{\Delta})^{1/2}}\sinh\tau\right] \\ -\phi_2+2c\sqrt{2}\,\phi_1\left[\dfrac{\cosh\tau}{(v^2-c^2+1+\sqrt{\Delta})^{1/2}}+\dfrac{\sinh\tau}{(c^2-1-v^2+\sqrt{\Delta})^{1/2}}\right] \\ \phi_1+2c\sqrt{2}\,\phi_2\left[\dfrac{\cosh\tau}{(v^2-c^2+1+\sqrt{\Delta})^{1/2}}+\dfrac{\sinh\tau}{(c^2-1-v^2+\sqrt{\Delta})^{1/2}}\right] \end{pmatrix},$$

$$\lambda^2=\begin{pmatrix} (c^2+1-v^2+\sqrt{\Delta})(\sqrt{\Delta}-v^2+c^2-1)^{1/2}+(c^2+1-v^2-\sqrt{\Delta})(v^2-c^2+1+\sqrt{\Delta})^{1/2} \\ 2\phi_1[(\sqrt{\Delta}-v^2+c^2-1)^{1/2}+(v^2-c^2+1+\sqrt{\Delta})^{1/2}] \\ 2\phi_2[(\sqrt{\Delta}-v^2+c^2-1)^{1/2}+(v^2-c^2+1+\sqrt{\Delta})^{1/2}] \end{pmatrix},$$

$$\lambda^3=\begin{pmatrix} (c^2+1-v^2+\sqrt{\Delta})+(c^2+1-v^2-\sqrt{\Delta})\dfrac{(v^2-c^2+1+\sqrt{\Delta})^{1/2}}{(c^2-1-v^2+\sqrt{\Delta})^{1/2}}\sin\tau \\ \dfrac{-\phi_2}{c\sqrt{2}}(v^2-c^2+1+\sqrt{\Delta})^{1/2}\cos\tau+2\phi_1\left[1+\left(\dfrac{v^2-c^2+1+\sqrt{\Delta}}{c^2-1-v^2+\sqrt{\Delta}}\right)^{1/2}\sin\tau\right] \\ \dfrac{\phi_2}{c\sqrt{2}}(v^2-c^2+1+\sqrt{\Delta})^{1/2}\cos\tau+2\phi_2\left[1+\left(\dfrac{v^2-c^2+1+\sqrt{\Delta}}{c^2-1-V^2+\sqrt{\Delta}}\right)^{1/2}\sin\tau\right] \end{pmatrix},$$

$$\lambda^4=\begin{pmatrix} \dfrac{\epsilon c\sqrt{2}(c^2+1-v^2+\sqrt{\Delta})}{(c^2-1-v^2+\sqrt{\Delta})^{1/2}} \\ -\phi_2+2\phi_1\dfrac{\epsilon c\sqrt{2}}{(c^2-1-v^2+\sqrt{\Delta})^{1/2}} \\ \phi_1+2\phi_2\dfrac{\epsilon c\sqrt{2}}{(c^2-1-v^2+\sqrt{\Delta})^{1/2}} \end{pmatrix},$$

$$\lambda^5=\begin{pmatrix} (c^2+1-v^2+\sqrt{\Delta})\left(\dfrac{\sqrt{\Delta}-v^2+c^2-1}{\sqrt{\Delta}+v^2-c^2+1}\right)^{1/2}\cosh\tau+(c^2+1-v^2-\sqrt{\Delta}) \\ \dfrac{-\phi_2}{c\sqrt{2}}(\sqrt{\Delta}-v^2+c^2-1)^{1/2}\sinh\tau+2\phi_1\left[1+\left(\dfrac{\sqrt{\Delta}-v^2+c^2-1}{\sqrt{\Delta}+v^2-c^2+1}\right)^{1/2}\cosh\tau\right] \\ \dfrac{\phi_1}{c\sqrt{2}}(\sqrt{\Delta}-v^2+c^2-1)^{1/2}\sinh\tau+2\phi_2\left[+1\left(\dfrac{\sqrt{\Delta}-)v^2+c^2-1}{\sqrt{\Delta}+v^2-c^2+1}\right)^{1/2}\cosh\tau\right] \end{pmatrix},$$

$$\lambda^6=\begin{pmatrix} \dfrac{\epsilon c\sqrt{2}(c^2+1-v^2+\sqrt{\Delta})}{(v^2-c^2+1+\sqrt{\Delta})^{1/2}} \\ -\phi_2+2\phi_1\dfrac{\epsilon c\sqrt{2}}{(v^2-c^2+1+\sqrt{\Delta})^{1/2}} \\ \phi_1+2\phi_2\dfrac{\epsilon c\sqrt{2}}{(v^2-c^2+1+\sqrt{\Delta})^{1/2}} \end{pmatrix},$$

where τ is an arbitrary function of ϕ_i, $i=0,1,2$, and

$$v^2=\phi_1^2=\phi_2^2,\quad \Delta=(v^2-c^2+1)^2+4c^2.$$

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Some rigorous results concerning spectral theory for ideal MHD

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Spectral theory for linear ideal MHD is laid on a firm foundation by defining appropriate function spaces for the operators associated with both the first- and second-order (in time and space) partial differential operators. Thus, it is rigorously established that a self-adjoint extension of $F(\xi)$ exists. It is shown that the operator L associated with the first-order formulation satisfies the conditions of the Hille–Yosida theorem. A foundation is laid thereby within which the domains associated with the first- and second-order formulations can be compared. This allows future work in a rigorous setting that will clarify the differences (in the two formulations) between the structure of the generalized eigenspaces corresponding to the marginal point of the spectrum $\omega = 0$.

I. INTRODUCTION

The purpose of this report is twofold: (1) to offer to the applied mathematician and theoretically inclined mathematical physicist a self-contained presentation of some rigorous theorems about the operators of linear ideal MHD (linearized Lundquist equations) in a bounded toroidal domain, and (2) to hopefully attract experts on spectral theory and hyperbolic equations to pitch in a hand towards resolving some of the difficult open problems remaining concerning the spectrum of the linearized operators and their connection with the time evolution of the first-order Lundquist equations, by recasting these problems precisely in the context of the appropriate functional spaces.

Concretely speaking, this report was motivated by its having been pointed out[1] that there exists an apparent gap in the literature on the linearized $F(\xi)$ introduced by Bernstein *et al.*,[2] which has long been known to be symmetric, as to whether a self-adjoint extension of the latter exists. As the author realized this result was an easy extension of his previous work,[3] he set out to exposit this in the present report. However, at that juncture his attention was drawn to a long unresolved problem introduced by Grad, as to the relation of the infinitesimal generator and spectrum of the original first-order Lundquist equations with that of the second-order system obtained therefrom by Bernstein *et al.*[2] Thus he was motivated to also present herein a self-contained proof of the existence of a semigroup solution to the linearized Lundquist equations and to thereby provide a concrete and rigorous setting within which the semigroup generated by them could be compared to the evolution equation associated with $F(\xi)$. Some preliminary remarks as to the comparison of the domains of the first- and second-order operators are made at the end of this paper.

We now pass to a more detailed account of what will be done in this report and stop along the way to survey the known results.

The Lundquist equations, or ideal MHD equations, constitute a first-order "quasi" symmetric hyperbolic system,[4] supplemented by the condition $\nabla\cdot B = 0$. We say "quasi" because (see Sec. IV C), in general, it is only after the condition $\nabla\cdot B = 0$ is imposed that the coefficient matrices are symmetric. In the context of nuclear fusion research they have traditionally been used to model the evolution of a plasma in a toroidal shell. They are supplemented and coupled with a set of pre-Maxwell equations when the plasma is surrounded by a vacuum region. If, however, the plasma is allowed to extend to the boundary, one obtains a so-called characteristic mixed initial boundary value problem. For the nonlinear case, even locally in time, no proof of the existence of solutions exists at the present time, and has appeared only very recently for the characteristic mixed initial boundary value for the Euler equations of compressible fluid dynamics in Ref. 5.

A linearization of the nonlinear equations around an equilibrium is beset with many difficulties since solutions to the equilibrium equations almost certainly do not exist in the absence of symmetry, as was convincingly demonstrated by Grad.[6] Therefore the following account, which deals with these linearized equations, will only be well founded for asymmetric perturbations of a symmetric equilibrium and needs, as does all the literature on the subject, to be carefully interpreted in the case of asymmetric equilibria. For an interesting discussion of these points see Ref. 1.

We would like to point out that for axisymmetric perturbations of axisymmetric equilibria an investigation along rigorous mathematical lines of the spectrum of $F(\xi)$ has been carried out in Refs. 7 and 8. Also a comprehensive survey paper of results on the spectrum due to Hameiri has been carried recently in a paper by the latter.[9]

In 1958, Bernstein *et al.*[2] derived, by introducing a Lagrangian displacement ξ in the original first-order Lundquist equations, a second-order symmetric operator $F(\xi)$ whose non-negativeness allegedly provided necessary and sufficient conditions for stability. It was soon noted, however, due to the presence of essential spectrum extending to and including the origin, that $F(\xi)\geqslant 0$ would be associated with nonexponential growth of the solution.[10] Goedbloed

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and Sakanaka[11] then formulated a modified energy principle, also referred to as the σ-stability principle, which, by avoiding difficulties at the origin, truly does provide necessary and sufficient conditions for a solution of $\rho\ddot{\xi} = F(\xi)$ to be σ-stable, which means that $\|\sqrt{\rho}\,\xi\|_2 \leqslant c \exp \sigma t$. This σ-stability principle was put on a firm mathematical foundation in Ref. 3. There, existence of solutions of $\rho\ddot{\xi} = F(\xi)$ in the form of a evolutionary variational problem following the work of Lions–Magenes,[12] was also established. A second-order semigroup approach to establishing existence for the same equations was outlined in Ref. 13, but all details have not appeared as of this writing.

It is well known that a complete resolution of an operator through its spectrum exists only for self-adjoint operators through the so-called spectral theorem. For operators that are merely symmetric but possessing no self-adjoint extension, the spectral problem is not well posed and its connection with the time evolution of the solution of the associated "generalized wave equation" is hard to interpret.

In the first part of this report we will show how machinery largely developed in Ref. 3 can be used to establish the existence of a self-adjoint extension of $F(\xi) + \lambda I$ for an appropriate λ. As far as the author can tell without adding a multiple of the identity to $F(\xi)$ it is indeed not possible to find a self-adjoint extension. Moreover, due to the boundary conditions on ξ, the appropriate multiple must be determined so as not only to make $F(\xi)$ positive but make its associated quadratic form coercive over a certain norm. Of course, loosely speaking, the spectrum of $F(\xi)$ can be thought of as merely a translation of the spectrum of $F(\xi) + \lambda I$. We will investigate the self-adjoint extension of $F(\xi)$, both in the context of the so-called diffuse pinch and sharp boundary models.

As pointed out by Grad[14] and more recently in Ref. 7, the second-order formulation in terms of $F(\xi)$ and the original formulation as a first-order system are not equivalent. Indeed the latter is the more fundamental and results about the former must be interpreted in that light. For completeness and as this problem was an important motivation for writing this report we provide a brief account.

The original first-order system can be written following the notation in Ref. 1:

$$v_t = L_1 \bar{v}, \tag{1}$$

$$\bar{v}_t = L_2 v, \tag{2}$$

where u is the fluid velocity, $\bar{v} = (p, B)$, scalar pressure and magnetic field. Introducing a Lagrangian displacement through

$$\frac{\partial}{\partial t}\xi(r_0,t) = v(r_0,t), \tag{3}$$

we then find by integrating that

$$\bar{v}(r_0,t) = L_2(\xi(r_0,t)) + (v(r_0,0) - L_2\xi(r_0,0)). \tag{4}$$

Thus if

$$\bar{v}(r_0,0) - L_2\xi(r_0,0) = 0, \tag{5}$$

we obtain from (1)

$$\xi_{tt} = L_1 L_2 \xi = F\xi, \tag{6}$$

which is the second-order formulation of Bernstein *et al.*[2] To illustrate (but not exhaust) the difficulties in passing from (1) and (2) to (6), note that (3) is artificial. An important class of initial perturbations referred to in Ref. 1 as the anholonomic ones consist precisely on those (u_0, v_0) that are not accessible from an equilibrium through a smooth displacement.

Another approach would be to differentiate (1) and substitute from (2) to obtain

$$v_{tt} = L_1 L_2 v = Fv. \tag{7}$$

However,[1] the only initial values of u, u_t that are relevant are those for which we can determine v from the relationship

$$v_t|_{t=0} = L_1 \bar{v}|_{t=0}. \tag{8}$$

In this report we hope to make a step towards the better understanding of the difference between the first- and second-order formulations by defining domains for both that we conjecture are as close as possible. This is so, as we will see, because the domain we will introduce for the second-order formulation is the domain of the square root of $F(\xi) + \lambda I$.

Further remarks could be made about the special difficulties in comparing the spectrum at the origin for the first- and the second-order formulations. For this we refer the reader to Ref. 1.

In the second part of this report we discuss the first-order system. Frequently this system is coupled with pre-Maxwell equations in a vacuum region surrounding the plasma. If however, the plasma is allowed to extend to the walls (diffuse pinch), one obtains an initial boundary value problem with characteristic boundary of constant multiplicity. A general theory does exist for such problems in the linear case, see Ref. 15 for an up-to-date account and recent developments. However, the boundary conditions $B \cdot n = 0$ on $\delta\Omega$ turns out not to be "admissible" in the general theory. So a slight modification of this theory is needed. We discuss this in a general way in Sec. IV C.

We will give here a self-contained proof of the existence of a linear semigroup solution to the characteristic initial boundary value problem assuming only the Hille–Yosida theorem.[16] The assumptions on the coefficients we will make will not be the most general possible. We note that the condition $\nabla \cdot B = 0$ for the system of Lundquist equations is nonstandard. For a smooth enough solution it will be satisfied for all time if satisfied initially. However, for a clear understanding of the relationship of the spectral problem with the time evolution of the system it is important to include it in the domain of the infinitesimal generator.

An advantage of a semigroup solution is that it gives a framework where we can appeal to the so-called spectral mapping theorems to relate the time evolution of the solution through the spectrum of the associated semigroup to the exponentiated spectrum of its infinitesimal generator. This last remark is especially relevant for the Lundquist equations linearized around a nonstatic equilibrium. There, too, is a second-order formulation of the stability problem,[17] however, in that case it is not a self-adjoint one and this further complicates an assessment of the relationship of the

study of the spectrum of the second-order operators with the time evolution of the first-order system.

II. EQUATIONS AND BOUNDARY CONDITIONS

Linearizing the Lundquist equations[2] of ideal MHD around a static ($u=0$) equilibrium that satisfies

$$\nabla p_0 = (\nabla\times B_0)\times B_0, \tag{9}$$

$$\nabla\cdot B_0 = 0, \tag{10}$$

yields the system

$$(1)\quad \rho_0\frac{\partial v}{\partial t} = -\nabla p + \nabla\times B_0\times B + \nabla\times B\times B_0, \tag{11}$$

$$(2)\quad \frac{\partial B}{\partial t} = \nabla\times(v\times B_0), \tag{12}$$

$$(3)\quad \frac{\partial p}{\partial t} = -\gamma p_0\nabla\cdot v - v\cdot\nabla p_0 \tag{13}$$

$$(4)\quad \nabla\cdot B = 0, \tag{14}$$

for the variables

$$\begin{pmatrix} v \\ p \\ B \end{pmatrix}.$$

Here we have denoted equilibrium quantities with the subscript 0.

When the plasma region Ω_p extends to the wall (diffuse pinch) the boundary conditions for the equilibrium equations are

$$B_0\cdot n = 0 \quad \text{on } \delta\Omega_p = \delta\Omega, \tag{15}$$

$$p = c \quad \text{on } \delta\Omega_p, \tag{16}$$

and, for the first-order system,

$$B\cdot n = 0 \quad \text{on } \delta\Omega, \tag{17}$$

$$v\cdot n = 0 \quad \text{on } \delta\Omega. \tag{18}$$

When the plasma region does not extend to the wall (sharp boundary model) in the vacuum region Ω_v surrounding the plasma, we introduce a vector potential for B, $\nabla\times A = B$, with the gauge condition $\nabla\cdot A = 0$ (see Ref. 18 for details), and then obtain in Ω_v the equations

$$\nabla\times\nabla\times\dot{A} = 0, \tag{19}$$

$$\nabla\cdot\dot{A} = 0, \tag{20}$$

and the boundary conditions

$$n_0\cdot\dot{A} = n_0\times(v\times B_0^p), \tag{21}$$

$$-\gamma p_0\nabla\cdot v + B_0^p\cdot(\nabla\times(v\times B_0^p) + v\cdot\nabla B_0^p) = B_0^v\cdot(\nabla\times A + v\cdot\nabla B_0^v), \quad \text{on } \Gamma_p \tag{22}$$

and

$$n\times\dot{A} = 0 \quad \text{on } \Gamma_v. \tag{23}$$

For the unique determination of $\dot{A}$ in a toroidal region we must also impose a flux condition

$$\int_{\Gamma_v}\dot{A}\cdot n\,ds = \dot{\gamma}(t). \tag{24}$$

From these equations we may derive, by introducing a Lagrangian displacement ξ satisfying

$$\frac{\partial\xi}{\partial t}(r_0,t) = v(r_0,t), \tag{25}$$

the equations

$$\rho_0\frac{\partial^2\xi}{\partial t^2} = \nabla(\gamma p_0\nabla\cdot\xi + \xi\cdot\nabla p_0) + \nabla\times B_0\times\nabla\times(\xi\times B_0) - B\times\nabla\times\nabla\times(\xi\times B_0) =: F(\xi), \quad \text{in } \Omega_p, \tag{26}$$

$$\nabla\times\nabla\times A = 0, \quad \text{in } \Omega_v, \tag{27}$$

$$\nabla\cdot A = 0, \quad \text{in } \Omega_v, \tag{28}$$

$$-\gamma p_0\nabla\cdot\xi + B_0^p\cdot(\nabla\times(\xi\times B_0^p) + \xi\cdot\nabla B_0^p) = B_0^v\cdot(\nabla\times A + \xi\cdot\nabla B_0^v), \tag{29}$$

$$n_0\times A = (-n\cdot\xi)B_0^v, \quad \text{on } \Gamma_p, \tag{30}$$

$$n_0\times A = 0, \quad \text{on } \Gamma_v, \tag{31}$$

and the flux condition

$$\int_{\Gamma_v} A\cdot n\,ds = \sigma(t). \tag{32}$$

As described in Refs. 3 and 18, these equations may be solved in the case of an inhomogeneous flux as in (32), by first solving them with a homogeneous flux

$$\int_{\Gamma_v} A\cdot n\,ds = 0, \tag{33}$$

and then adding to A a solution A' of the system

$$\nabla\times A' = 0, \tag{34}$$

$$\nabla\cdot A' = 0, \tag{35}$$

$$n_0\times A' = 0, \quad \text{on } \Gamma_p\cup\Gamma_v, \tag{36}$$

$$\int_{\Gamma_v} A'\cdot n\,ds = \sigma(t). \tag{37}$$

In the case of the diffuse pinch the equations are

$$\rho\frac{\partial^2\xi}{\partial t^2} = F(\xi), \tag{38}$$

$$\xi\cdot n = 0, \quad \text{on } \Gamma_p. \tag{39}$$

We now associate, as in Ref. 3, with the operator $F(\xi)$ a bilinear form

$$\begin{aligned} a(\xi,\tilde{\xi}) = \int_{\Omega_p}\{&\gamma p(\nabla\cdot\xi)(\nabla\cdot\tilde{\xi}) + \nabla\times(\xi\times B)\cdot\nabla\times(\tilde{\xi}\times B) \\ &- \nabla\times B\times\xi\cdot\nabla\times(\tilde{\xi}\times B) - (\nabla\cdot\xi)(\tilde{\xi}\cdot\nabla p)\}dx \\ &+ \int_{\Omega_v}\nabla\times A\cdot\nabla\times\tilde{A}\,d\cdot x \\ &- \int_{\Gamma_p}(\xi\cdot n)(\tilde{\xi}\cdot n) \\ &\times n\cdot\nabla\left(p + \frac{1}{2}|B_0^{p^2}| - \frac{1}{2}|B_0^{v^2}|\right)ds. \end{aligned} \tag{40}$$

We assume $n\cdot\nabla(p + \frac{1}{2}|B_0^{p^2}| - |B_0^{v^2}|) > 0$. Here A, $\tilde{A}$ are defined in terms of $\xi,\tilde{\xi}$ by solving the boundary value problem (27) and (28) subject to the boundary conditions (30) and (31) and the flux condition (33).

In the case of the diffuse pinch, the last two terms in the form are absent since $\xi\cdot n = \tilde{\xi}\cdot n = 0$ and the unique solution of the boundary value problem defined just above for A and

$\tilde{A}$ is zero. We will hereafter refer to the diffuse pinch as case 1, and the sharp boundary as case 2.

III. SELF-ADJOINT EXTENSIONS

In this section we will establish that the operator $F(\xi)$ defined by (26) has a self-adjoint extension. The nature of this extension is different in an essential way according as to whether we are in case 1 (diffuse pinch) or case 2 (sharp boundary). In both cases the extension we will use is the so called Friedrichs extension.

In case 1, the following general theorem (see Theorem X23, p. 177 of Ref. 19) will be needed.

Theorem 3.1: Let A be a positive symmetric operator and let $a(\psi,\phi) = \langle \psi, A\phi \rangle$, for $\psi,\phi \in D(A)$. Then a is a closable quadratic form and its closure $\hat{a}$ is the quadratic form of a unique self-adjoint operator $\hat{A}$. The operator $\hat{A}$ is a positive extension of A, and the lower bound of its spectrum is the lower bound of a. Further, $\hat{A}$ is the only self-adjoint extension of A whose domain is contained in the form domain of $\hat{a}$.

A few general remarks are in order about how we apply this theorem. First of all, in our case $A = F(\xi)$ is not necessarily a positive operator. To make it positive we must add a multiple λ of the identity to $F(\xi)$. Although we then satisfy all the conditions of the theorem, the closure of the form domain for

$$a_\lambda(\xi,\xi) = \langle F(\xi) + \lambda I(\xi), \xi \rangle \tag{41}$$

may not be such that all its elements satisfy $\xi \cdot n = 0$ on $\delta\Omega$. As we will see in the sequel, however, there is a value of λ sufficiently large (the one that makes the associated quadratic form coercive over a certain norm) for which the form domain of $\hat{a}_\lambda(\xi,\xi)$ does satisfy the boundary condition. Thus according to the general principle expounded in the theorem for this λ, the associated closed s.a. operator $\hat{F}(\xi) + \lambda I$, does incorporate the boundary condition $\xi \cdot n = 0$ in its domain.

Furthermore this theorem makes clear how we can justify in a rigorous way a vast physics literature that implicitly assumes that a lower bound for the quadratic form yields a lower bound for the spectrum of $F(\xi)$, a result that is not true for all extensions of $F(\xi)$. This theorem also is connected with the author's being able to justify in Ref. 3 the so-called modified energy principle. There, solutions to an associated evolutionary variational problem were constructed precisely in the form domain of $\hat{a}_\lambda$.

Case 2 (sharp boundary) is unorthodox. Indeed *a priori* it is not clear that the natural domain one would like to associate with $F(\xi)$ is not empty. This natural domain is

$$\{\xi \in H^1(\Omega):\ F(\xi) \in L^2(\Omega),\ \gamma p_0 \nabla\cdot\xi + B^p(\nabla\times(\xi\times B_0^p) + \xi\cdot\nabla B_0^p) = B_0^v\cdot(\nabla\times A + \xi\cdot\nabla B_0^v)\},\ \text{on } \Gamma_p. \tag{42}$$

Here A is defined in terms of ξ by satisfying (27), (28), (30), (31), and (33). Bernstein *et al.*[2] give a heuristic argument that this domain is not empty. Essentially they argue that as we do not alter A by changing the tangential component of ξ on Γ_p alone, so we may adjust this tangential component in order that (29) is satisfied. The justification of this argument, involving as it does the solution of a partial differential equation on a closed toroidal surface, does not appear to be straightforward.

The method we use to get around this difficulty is the following. With no *a priori* mention of the operator $F(\xi)$ we introduce the quadratic form $a(\xi,\xi) + \lambda(\xi,\tilde{\xi})$ through (40). The second half of the theorem quoted above then insures us of the existence of a self-adjoint extension $\hat{F}_\lambda(\xi) + \lambda I(\xi)$, which by general principles is defined on a dense subset of $L^2(\Omega_p)$ contained in the form domain of $\hat{a}(\xi,\tilde{\xi}) + \lambda(\xi,\tilde{\xi})$. By the nature of this extension we have

$$\hat{a}(\xi,\tilde{\xi}) + \lambda(\xi,\tilde{\xi}) = \langle \hat{F}_\lambda(\xi) + \lambda\xi, \tilde{\xi} \rangle. \tag{43}$$

On the other hand, Green's theorem implies

$$\hat{a}(\xi,\tilde{\xi}) + \lambda(\xi,\tilde{\xi}) = \langle \hat{F}_\lambda\xi + \lambda\xi, \tilde{\xi} \rangle + \int (\tilde{\xi}\cdot n) L(\xi,A)\,ds = 0, \tag{44}$$

where $L(\xi,A)$ is given by (29). As mentioned above, the set of $\tilde{\xi}$'s satisfying (44) are dense in $L^2(\Omega_p)$, hence in $H^1(\Omega_p)$. Thus the associated restrictions to the boundary $(\tilde{\xi}\cdot n)$, are clearly dense in $L^2(\Omega_p)$ by the trace theorems.

This then implies $L(\xi,A) = 0$. Hence by this indirect route we have established that there exist a dense set of ξ in $L^2(\Omega_p)$, which is in the domain defined by (42).

In the following we show that the conditions of the theorem are satisfied by the bilinear form (40), and that the form domain incorporates the relevant boundary conditions. Many details are omitted and can be found in Ref. 3.

Case 1 (diffuse pinch): In the following all derivatives are taken in the sense of distributions. The domain of $F^-(\xi)$ we take to be

$$D^-(F) = \{\xi \in H^2(\Omega) \mid \xi\cdot n = 0 \text{ on } \delta\Omega\}. \tag{45}$$

We introduce the form core

$$W^- = \{\xi \in H^1(\Omega_p^-),\ \xi\cdot n = 0 \text{ on } \Gamma_p\}, \tag{46}$$

with the norm

$$\|\xi\|_W^2 = \int_{\Omega_p} \{\gamma p(\nabla\cdot\xi)^2 + |\nabla\times(\xi\times B_0^p)|^2 + \lambda|\xi|^2\}dx, \tag{47}$$

and define

$$W = \{\xi\cdot n = 0 \text{ on } \Gamma_p \mid \xi, \nabla\cdot\xi, \nabla\times(\xi\times B_0^p) \in L^2(\Omega_p)\}. \tag{48}$$

It is easily seen that on $D^-(F)$, $a(\xi,\tilde{\xi}) = \langle F(\xi), \xi \rangle$. A standard density argument[12] allows us to show $\{C^1(\Omega_p),\ \xi\cdot n = 0 \text{ on } \Gamma_p\}$ is dense in W^- and W. Also $a(\xi,\tilde{\xi})$ is symmetric on W^- and there exist constants $c_1, c_2, \delta(c_1, c_2, \lambda)$ s.t.

$$c_1\|\xi\|_W^2 \leqslant a(\xi,\xi) + \delta\|\xi\|_W^2 \leqslant c_2\|\xi\|_W^2, \tag{49}$$

see Ref. 18.

The important point to check is that $a(\xi,\tilde{\xi})$ is a closed form that is equivalent to be completeness of W in the W norm defined in (47). This essentially reduces to checking that the boundary condition $\xi\cdot n = 0$ on Γ_p makes sense for elements in W. This is an easy consequence of the inequality[12]

$$\|\xi\cdot n\|_{H^{-1/2}(\Gamma)}^2 \leqslant c\{\|\xi\|_2^2 + \|\nabla\cdot\xi\|_2^2\}. \tag{50}$$

We may now apply Theorem (3.1) to show that $F_\lambda^-(\xi)$ has

a self-adjoint extension to $F_\lambda(\xi)$ with domain given by

$$D(F_\lambda) = \{\xi \in W \mid F(\xi) \in L^2(\Omega)\}, \tag{51}$$

and that on $D(F_\lambda)$, $a(\xi,\tilde{\xi}) = \langle F_\lambda(\xi), \tilde{\xi} \rangle$. Here we have defined

$$F_\lambda(\xi) = F(\xi) + \lambda I(\xi). \tag{52}$$

Case 2 (sharp boundary): We first introduce some relevant function spaces, in the notation of Ref. 3. Recalling the Hodge decomposition theorem, if $V = (v_1, v_2, v_3) \in L^2(\Omega)$, then there exists

$$V_1 \in \overline{V}_1, \quad V_2 \in \overline{V}_2, \quad V_3 \in \overline{V}_3, \tag{53}$$

such that

$$V = V_1 + V_2 + V_3 \tag{54}$$

or

$$L^2(\Omega) = \overline{V}_1 + \overline{V}_2 + \overline{V}_3, \tag{55}$$

and the decomposition is orthogonal, where

$$\overline{V}_1 = \{\nabla\phi \mid \phi \in H_0^1(\Omega)\}, \tag{56}$$

$$\overline{V}_2 = \{\nabla \times v \mid v \in L^2(\mathrm{rot})(\Omega)\}, \tag{57}$$

$$L^2(\mathrm{rot})(\Omega) = \{V \in L^2(\Omega) \mid \nabla \times v \in L^2(\Omega)\}, \tag{58}$$

$$\overline{V}_3 = \{h \mid \nabla \times h = 0,\ \nabla \cdot h = 0 \text{ in } \Omega,\ n \times h = 0 \text{ on } \delta\Omega\}. \tag{59}$$

All derivatives above are taken in the sense of distributions.

We define W as the closure in the W norm of $W^- = H^1(\Omega_p)$, where

$$\|\xi\|_W^2 = \int_{\Omega_p} \{\gamma p(\nabla \cdot \xi)^2 + |\nabla \times (\xi \times B_0^p)|^2 + \lambda |\xi|^2\} dx + \int_{\Omega_v} |\nabla \times A|^2.$$

Here A is defined in terms of ξ by solving the boundary value problem

$$\nabla \times \nabla \times A = 0, \tag{60}$$

$$\nabla \cdot A = 0, \tag{61}$$

$$n \times A = (-n \cdot \xi) B_0^v, \quad \text{on } \Gamma_p, \tag{62}$$

$$n \times A = 0, \quad \text{on } \Gamma_v, \tag{63}$$

$$\int_{\Gamma_p} A \cdot n \, ds = 0. \tag{64}$$

The fundamental properties of W are given in Theorem 4.3 of Ref. 3, which we recall here.

Theorem 3.2: W is a Hilbert space of a vector-valued function ξ for which

(1) $\nabla \times (\xi \times B_0^p)$, $\nabla \cdot \xi$, $\xi \in L^2(\Omega_p)$,

(2) $(\xi \cdot n) B_0^v \in H^{-1/2}(\Gamma_p)$,

and (3) the boundary value problem defined by (60)–(64) for A has a solution for which $A \in L^2(\mathrm{rot})(\Omega_v) \cap \overline{V}_2(\Omega_v)$.

For the proof, see Ref. 3. Here we would like to give an elaboration of condition (3). However, we note, as will become clear from this elaboration, that (3) is actually a refinement of (2).

Consider the boundary value problem (60)–(64). In Theorem 4.1 of Ref. 3 the inequality

$$\|A\|_2 \leqslant c\{\|\nabla \times A\|_2 + \|n \times A\|_{H^{-1/2}(\Gamma)}\} \tag{65}$$

was established for $A \in L^2(\mathrm{rot})(\Omega) \cap \overline{V}_2(\Omega)$, where Ω is a possibly multiply connected domain. An inspection of the proof of this theorem reveals that if in addition

$$\nabla \times \nabla \times \mathrm{A} = 0,$$

then

$$\|A\|_2 \leqslant c\|n \times A\|_{H^{-1/2}(\Gamma)}. \tag{66}$$

This follows from the fact that if g is defined as in that theorem by

$$\nabla \times \nabla \times g = f, \tag{67}$$

$$\nabla \cdot g = 0, \quad \text{in } \Omega, \tag{68}$$

$$n \times g = 0, \quad \text{on } \Gamma_p \cup \Gamma_v, \tag{69}$$

$$\int_{\Gamma_p} g \cdot n \, ds = 0, \tag{70}$$

then

$$\int_\Gamma \nabla \times A \cdot \nabla \times g \, ds = 0, \tag{71}$$

and we refer the reader to the proof of Theorem 4.1 to see how this last equality implies (66).

A consequence of (66) is that a solution of (60)–(64) exists if $(n \cdot \xi) B_0^v$ and therefore $n \times A$ is in $H^{-1/2}(\Gamma_v)$. Here the condition

$$\int_{\Gamma_v} A \cdot n \, ds = 0$$

must be interpreted in the sense of duality

$$\langle A, n \rangle_{H^{-1/2}(\Gamma_v) \times H^{1/2}(\Gamma_v)} = 0. \tag{72}$$

Note, to write (72) we have used again the result, $A \in L^2(\Omega)$, $\nabla \cdot A = 0 \Rightarrow A \cdot n \in H^{-1/2}(\Gamma_p \cup \Gamma_v)$. However, the conditions $n \times A \in H^{-1/2}(\Gamma_p)$, $n \times A = 0$ on Γ_v do not suffice to ensure

$$\nabla \times A \in L^2(\Omega_v). \tag{73}$$

Thus what characterizes W is that $\xi \cdot n$ lies in a subset of $H^{-1/2}(\Gamma_p)$ for which (73) is satisfied. Whether this last fact entails further regularity for ξ in Γ_p and/or ξ on Γ_p is an open problem.

We can now apply again Theorem 3.1 to define the domain of the self-adjoint operator $F_\lambda(\xi)$ by

$$D(F_\lambda) = \{\xi \in W \mid a(\xi,\tilde{\xi}) = \langle F_\lambda(\xi), \tilde{\xi} \rangle\}.$$

The theorem guarantees that this domain is dense in $L^2(\Omega)$.

IV. FIRST-ORDER LUNDQUIST EQUATIONS: SEMIGROUP SOLUTIONS AND SPECTRAL MAPPING THEOREMS

To begin this presentation we make a change of variables that puts the Lundquist equations in canonical symmetric hyperbolic form

$$u_t = \sum_i A_i \frac{\partial}{\partial x_i} u + Bu, \tag{74}$$

u is an n-vector and the A_i are symmetric n–n-matrices. We do this in the following subsection.

A. Quasisymmetric hyperbolic form of equations

Let $\rho = (p/s)^{1/\gamma}$ and

$$\tilde{p} = (\gamma p_0)^{-1/2} p, \tag{75}$$

$$\tilde{v} = (\rho_0)^{1/2} v. \tag{76}$$

In the new variables the Lundquist equations linearized around an arbitrary equilibrium (static or nonstatic) can be rewritten as

$$\begin{aligned}\tilde{v}_t = &-\left(\frac{\gamma p_0^{1/2}}{\rho_0}\right)^{1/2}\nabla\tilde{p} + \frac{\gamma(p_0\rho_0)^{-1/2}}{2}\tilde{p}\nabla p_0 \\ &+ (\rho_0)^{-1/2}\nabla\times B\times B_0 + \rho_0^{-1/2}\nabla\times B_0\times B \\ &- v_0\cdot\nabla\tilde{v} + \frac{1}{2\rho_0}\tilde{v}v_0\cdot\nabla\rho_0 - \frac{\rho}{\rho_0^{1/2}}v_0\cdot\nabla v_0 - \tilde{v}\cdot\nabla v_0,\end{aligned} \tag{77}$$

$$B_t = \rho_0^{-1/2}\nabla\times(\tilde{v}\times B) - \tfrac{1}{2}\rho_0^{-3/2}[\nabla\rho_0\times(\tilde{v}\times B)], \tag{78}$$

$$\begin{aligned}\tilde{p}_t = &-\left(\frac{\gamma p_0}{\rho_0}\right)^{1/2}\nabla\cdot\tilde{v} + \frac{1}{2}(\gamma p_0\rho_0^3)^{1/2}\tilde{v}\cdot\nabla\rho_0 \\ &- (\gamma p_0\rho_0)^{-1/2}\tilde{v}\cdot\nabla p_0 \\ &- v_0\cdot\nabla\tilde{p} - \frac{1}{2(p_0\rho_0)^{1/2}}v_0\cdot\nabla p_0,\end{aligned} \tag{79}$$

$$S_t = -\rho_0^{-1/2}\tilde{v}\cdot\nabla S_0 - v_0\cdot\nabla S, \tag{80}$$

with principal part

$$\tilde{v}_t = -\left(\frac{\gamma p_0}{\rho_0}\right)^{1/2}\nabla\tilde{p} + \rho_0^{-1/2}\nabla\times B\times B_0 + \cdots, \tag{81}$$

$$B_t = \rho_0^{-1/2}\nabla\times(\tilde{v}\times B), \tag{82}$$

$$\tilde{p}_t = -\left(\frac{\gamma p_0}{\rho_0}\right)^{1/2}\nabla\cdot\tilde{v} + \cdots, \tag{83}$$

$$S_t = -v_0\cdot\nabla S. \tag{84}$$

To this set of equations we must add the condition

$$\nabla\cdot B = 0. \tag{85}$$

In this form with the help of a few vector identities the symmetry of the $\tilde{A}_i$ is easily ascertained directly when $v_0 = 0$. We next discuss in a general way the relationship of the semigroup solutions we will define with the spectrum of their infinitesimal generators. The discussion will apply whether the underlying equilibrium state is static or nonstatic (with flow). We hereafter drop the tilde in the perturbed quantities.

B. Remarks on spectral mapping theorems

The assumed smoothness of p_0, ρ_0, and B_0 allow us to define all the spatial differential operators arising in (74) in the sense of distributions. Let

$$u = \begin{pmatrix} v \\ B \\ p \\ S \end{pmatrix}$$

and let

$$Lu = A_i\frac{\partial}{\partial x_i}u + Bu,$$

where the derivatives are taken in the sense of distributions and A_i and B are determined by (77)–(80).

A natural definition for the domain of L would be

$$D(L) = \begin{Bmatrix} u\in\{L^2(\Omega)\}^8: & \nabla\cdot B = 0, & Lu\in\{L^2(\Omega)\}^7 \\ v\cdot n = 0 \text{ on } \delta\Omega, & B\cdot n = 0 \text{ on } \delta\Omega & \end{Bmatrix}. \tag{86}$$

We hereafter will use the shorthand $u\in L^2(\Omega)$ instead of $u\in\{L^2(\Omega)\}^8$. On this domain, however, we conjecture that L is not a closed operator. This is due to the failure in general of the condition

$$\frac{B' + B^*}{2} - \frac{\partial}{\partial x_i}A_i \geqslant 0. \tag{87}$$

Thus we will instead consider

$$L + \bar{\lambda}I,$$

where $\bar{\lambda}$ is determined so as to ensure that $L + \bar{\lambda}I$ is a closed operator if $\bar{\lambda} > \lambda_0$. It can also easily be shown that for the proper choice of λ_0 all the domains of the associated $L + \bar{\lambda}I$ are the same. Thus, for the purposes of this preliminary discussion, without loss of generality, we fix a particular $\bar{\lambda} > \lambda_0$.

$L + \bar{\lambda}I$ will be shown to be the infinitesimal generator of a semigroup denoted $T_{\bar{\lambda}}(t)$. Formally

$$e^{(L+\bar{\lambda}I)t} = T_{\bar{\lambda}}(t) = e^{\bar{\lambda}t}e^{Lt} = e^{\bar{\lambda}t}T(t), \tag{88}$$

where $T(t)$ is the solution to original system (74). Thus for a particular initial data u_0 the solution of

$$u_t + \sum A_i\frac{\partial}{\partial x_i}u + Bu = 0, \tag{89}$$

$$u(x,0) = u_0 \tag{90}$$

is

$$u(x,t) = e^{-\bar{\lambda}t}T_{\bar{\lambda}}(t)u_0, \tag{91}$$

for any $u_0\in D(L + \bar{\lambda}I)$. We recall, as is well known,[16] that the set of λ's in the spectrum of $T(t) = e^{-\bar{\lambda}t}T_{\bar{\lambda}}(t)$ are contained in a strip in the complex plane, $\sigma_- < \mathrm{Re}\,\lambda < \sigma_+$. Once we have shown that $L + \bar{\lambda}I$ generates the semigroup $T_{\bar{\lambda}}(t)$, the spectral mapping theorems (see Ref. 20, pp. 44–48) will guarantee that the following set inclusions hold:

$$\{e^{\sigma(L+\bar{\lambda}I)t}\}\subset\sigma(T_{\bar{\lambda}}(t)), \tag{92}$$

therefore

$$e^{-\bar{\lambda}t}\{e^{(\sigma(L+\bar{\lambda}I)t}\}\subset e^{-\bar{\lambda}t}\sigma(T_{\bar{\lambda}}(t)), \tag{93}$$

but

$$\sup_{\bar{\sigma}\in\sigma(L+\bar{\lambda}I)} e^{\sigma(L+\bar{\lambda}I)t} \leqslant \|T_{\bar{\lambda}}(t)\|. \tag{94}$$

And

$$\sup\{|\lambda|\,|\,\lambda\in e^{-\bar{\lambda}t}\sigma(T_{\bar{\lambda}}(t))\} \leqslant e^{-\bar{\lambda}t}\|T_{\bar{\lambda}}(t)\|, \tag{95}$$

and therefore

$$\sup_{\sigma\in(L+\bar{\lambda}I)} e^{-\bar{\lambda}t}e^{\sigma(L+\bar{\lambda}I)t} \leqslant e^{-\bar{\lambda}t}\|T_{\bar{\lambda}}(t)\|. \tag{96}$$

Equality holds, for instance, when $T_{\bar{\lambda}}$ is self-adjoint, which it is not in our case.

The foregoing inclusions are the only general statements that can be made in an abstract way as to the relation of the spectrum of the infinitesimal generator and the time evolution of the associated semigroup. They show that we cannot expect to get from the spectrum of the infinitesimal gener-

ator necessary and sufficient conditions for stability. This is, moreover, not due to the lack of regularity of the semigroup solution as the problem exists even for analytic semigroups.[21]

The spectral mapping theorems do, however, justify, through (96), the procedure of deriving necessary conditions for stability or, put a different way, sufficient conditions for instability from the knowledge of the range of the spectrum of $L+\bar{\lambda}I$.

When linearizing around a static equilibrium we can say a good deal more, at least in a heuristic fashion, about the time evolution of the Lundquist equations by considering the spectrum of the self-adjoint second-order operator $F(\xi)$, see (26), which arises when we integrate the system (2) so as to obtain an equation for ξ alone. Heuristically, we would expect that any exponential growth of the semigroup $T(t)$ would correspond to a negative element in the spectrum of $F(\xi)$. However, there are difficulties in justifying this argument, as we pointed out in the Introduction, which we will not resolve here beyond the comments made at the end of this work as to the comparison of the domains of $F(\xi)$ and L. What we would like to stress at this juncture is that when linearizing around a nonstatic equilibrium where there is no self-adjoint second-order formulation, a sharper version of the spectral mapping theorems may prove the most viable route towards a better understanding of the relation of the spectrum of L (or $L+\bar{\lambda}I$) to the time evolution of the semigroup $T(t)$ [or $T_{\bar{\lambda}}(t)$].

We now turn to the proof of the existence of a semigroup solution. We will consider separately the cases (1) linearization around a static equilibrium, (2) linearization around an equilibrium with flow, and (3) incompressible plasmas. Before we do this, we will make some general remarks about the nonapplicability of the general theory of maximal positive boundary data for symmetric positive systems to our case. These remarks may be of interest only to those already familiar with the theory and may be skipped without loss of continuity.

We consider the static case separately as opposed to a special case of the nonstatic case in order to facilitate future work regarding the comparison of the first- and second-order operators and associated questions mentioned previously.

C. On the inapplicability of general theory for symmetric positive systems

This section is intended for those who are familiar with the theory of maximal positive boundary data for symmetric positive systems.

We recall the general principle. Suppose we denote by $N(x)$ the linear subspace in which the vector

$$\begin{pmatrix} v \\ p \\ B \\ S \end{pmatrix}$$

must lie in if it is to satisfy the boundary condition at x. Here N is called maximal positive if

$$\langle A_n(x)w,w\rangle \geqslant 0, \quad \forall x\in\delta\Omega,\ w\in N(x), \tag{97}$$

where

$$A_n = A_\nu n_\nu, \tag{98}$$

and if N cannot be enlarged while preserving (97). Note that clearly $\ker A_n \subset N$.

Now a simple calculation shows that the matrix A_n for the system (77)–(80) has the form

$$\begin{vmatrix} (-n\cdot v_0) & -(\gamma p_0/\rho_0)^{1/2} n & \rho_0^{-1/2}[(n\cdot B_0) - n(B_0\cdot)] & 0 \\ -(\gamma p_0/\rho_0)^{1/2} n & (-v_0\cdot n) & & 0 \\ \rho_0^{-1/2}[B_0\cdot n) - B_0(n\cdot)] & & -(v_0\cdot n) + v_0(n\cdot) & 0 \\ 0 & 0 & 0 & -v_0\cdot n \end{vmatrix} \begin{pmatrix} \tilde{v} \\ \tilde{p} \\ \dot{B} \\ S \end{pmatrix}. \tag{99}$$

The above matrix is so far completely general. That is, we have not yet imposed any boundary conditions on the equilibrium quantities v_0, p_0, and B_0. We have used the notation $B_0(n\cdot)$ to denote the operator submatrix that acts on $w=(w_1,w_2,w_3)$ through

$$(B^i_0 n^j)(w) = B^i_0 n^j w_j. \tag{100}$$

The transposed matrix operator is

$$B^j_0 n_i, \tag{101}$$

which we denote by

$$n(B_0\cdot). \tag{102}$$

The matrix (99) is manifestly symmetric except for the expression

$$-(v_0\cdot n) + v_0(n\cdot), \tag{103}$$

whose transpose is

$$(-v_0\cdot n) + (n(v_0\cdot)). \tag{104}$$

We see that (103) and (104) are not generally equal. This is why we refer to (77)–(80) as a quasisymmetric hyperbolic system. When we restrict the action of (99) to elements B satisfying $B\cdot n = 0$ the symmetry is salvaged. Here $B\cdot n = 0$ is valid for the B^j_s that are *subjected to the condition* $\nabla\cdot\mathbf{B} = 0$.

Note, however, that *for static equilibria* $v_0 = 0$, and the symmetry holds even without $\nabla\cdot\mathbf{B} = 0$.

We now turn to the discussion of the matrix (99) when it operates on the boundary. There the conditions $n\cdot v_0 = n\cdot B_0 = 0, p_0 = c$ must be imposed. It is to the corresponding simplified matrix and its operator kernel that we will now refer. Again, even at the boundary, this matrix is only symmetric when acting on a domain consisting of u's, $u=(\tilde{v},\tilde{p},B)$, for which $\nabla\cdot B = 0$. Even on this restricted domain the conditions (97) of the general theory do not hold

however. To see this consider an element $u=(\tilde{v},\tilde{p},B,S)$, which satisfies

$$n\cdot\tilde{v}=0, \tag{105}$$

$$\frac{1}{\rho_0^{1/2}}(B_0\cdot B)+\left(\frac{\gamma p_0}{\rho_0}\right)^{1/2}\tilde{p}=0. \tag{106}$$

It is easily seen that such u satisfy $u\in\mathrm{Ker}\,A_n$. However, although $\tilde{v}\cdot n=v\cdot n=0$, (106) does not imply that $B\cdot n=0$, thus

$$\mathrm{Ker}\,A_n\not\subset N(x). \tag{107}$$

Of course reinstating the condition $\nabla\cdot B=0$ and its "characteristic" equivalent $n\cdot B=0$,

$$\mathrm{Ker}\,A_n\subset N(x),$$

if we interpret A_n as acting only on this subspace. Note that given the change of variables (75) and (76), (106) is the linearized version of the condition

$$p+B^2/2=c, \tag{108}$$

which thus appears to be a more natural boundary condition than the traditionally imposed one $B\cdot n=0$.

D. Existence of semigroup solutions

We first recall the following definition.

Definition: A semigroup $T(t)$, $0\leqslant t<\infty$, of bounded operators is said to be a continuous C_0 semigroup in a Banach space x if

$$\lim_{t\downarrow 0}T(t)x=x,\quad \text{for every } x\in X.$$

These remarks may be of interest only to those unfamiliar with the theory and may be skipped without loss of continuity. We also recall the Hille–Yosida theorem.

Theorem 4.1: An operator $A: X\to X$ is the generator of a semigroup of bounded operators $T(t)$ satisfying

$$\|T(t)\|\leqslant ce^{\omega t},$$

if and only if (1) A is a closed operator with dense domain, (2) the resolvent set $\rho(A)$ of A contains (ω,∞), and (3) $\|(\lambda I-L)^n\|\leqslant M/|\lambda-\omega|^n$. Furthermore, if $M=1$, (3) can be deduced from

$$(3')\quad \|\lambda I-A\|\leqslant 1/|\lambda-\omega|. \tag{109}$$

We will show that the conditions of the theorem are verified for the operator $L+\bar{\lambda}I$ defined by (77)–(80) on an appropriate domain. Details will be given only for linearization around a static equilibrium.

Case A (static equilibrium): X, the underlying Hilbert space, will be defined by

$$X=\{\tilde{v}=(u,p,B)\,|\,u\in L^2(\Omega),\ \nabla\cdot B=0\}. \tag{110}$$

Remark: Note that L maps $(\tilde{v},B,\tilde{p})$ to $(-,\nabla\times(\tilde{v}/\rho_0^{1/2}\times B_0),-)$. As

$$\nabla\cdot(\nabla\times(\tilde{v}/\rho_0^{1/2}\times B_0))=0, \tag{111}$$

$Lu\in X$, provided $Lu\in L^2(\Omega)$. Clearly the same holds for

$$Lu+\bar{\lambda}I; \tag{112}$$

$\bar{\lambda}$ will be determined by (77)–(80). We now define

$$D(L_{\bar{\lambda}})=\{u=(v,p,B)\,|\,u\in L^2(\Omega),\ L_{\bar{\lambda}}u\in L^2(\Omega),$$
$$\nabla\cdot B=0,\ v\cdot n=0,\ B\cdot n=0 \text{ on } \delta\Omega\}. \tag{113}$$

Clearly $D(L_{\bar{\lambda}})\in X$. Furthermore, if $\delta\Omega$ is smooth enough, say C^2, and we define

$$D^+(L_\lambda)=\{u=(v,p,B)\,|\,v\in C^1(\Omega),$$
$$\nabla p-\nabla\times B\times B_0\ \in C_1(\Omega),$$
$$\nabla\cdot B=0,\ \tilde{v}\cdot n=0,\ B\cdot n=0 \text{ on } \delta\Omega\},$$

then $D^+(L_{\bar{\lambda}})$ is dense in $D(L_{\bar{\lambda}})$ in the graph norm $\|L_{\bar{\lambda}}u\|$. To show this we will first need to show the following theorem.

Theorem 4.2: $L_{\bar{\lambda}}$ is a closed operator for sufficiently large $\bar{\lambda}$.

Proof: We first show that on the domain D^+, the following inequality holds for large λ:

$$\|L_{\bar{\lambda}}+\lambda u\|\geqslant c\|u\|. \tag{114}$$

For $u\in D^+$, this is a consequence of the symmetry of the A_i's and the boundary conditions $u\cdot n=B\cdot n=0$ on $\delta\Omega$. One reasons as follows: Let λ be real, consider

$$\langle(L+\lambda I)u,(L+\lambda I)u\rangle$$
$$=\|Lu\|^2+\lambda^2\|u\|^2+2\ \mathrm{Re}\ \lambda\langle Lu,u\rangle. \tag{115}$$

Now

$$\langle Lu,u\rangle=\left\langle A_i\frac{\partial}{\partial x_i}u+Bu,u\right\rangle \tag{116}$$

$$=\left\langle\frac{\partial}{\partial x_i}u,A_iu\right\rangle+\langle Bu,u\rangle \tag{117}$$

$$=-\left\langle u,\frac{\partial}{\partial x_i}(A_iu)\right\rangle+\langle Bu,u\rangle \tag{118}$$

$$=-\left\langle u,\left(\frac{\partial}{\partial x_i}A_i\right)u\right\rangle-\left\langle u,A_i\frac{\partial}{\partial x_i}u\right\rangle$$
$$+\langle Bu,u\rangle. \tag{119}$$

Here in the second step we have used the symmetry of the A_i; in the third, the integration by parts, the boundary terms dropped out because

$$\int_\Gamma\langle A_in_iu,u\rangle ds=0. \tag{120}$$

Specifically the boundary terms that arise are

$$\tilde{p}(\tilde{v}\cdot n),\{(\tilde{v}\times B_0)\times B\}\cdot n. \tag{121}$$

The second term can be written

$$(\tilde{v}_0\cdot B)B_0\cdot n-(B_0\cdot B)\tilde{v}\cdot n, \tag{122}$$

which vanishes by virture of (17) and (18). It is noteworthy that the boundary condition

$$B\cdot n=0$$

was not used to establish (118). Thus, from (118) we obtain

$$\left|2\,\mathrm{Re}\left\langle A_i\frac{\partial}{\partial x_i}u,u\right\rangle+2\mathrm{Re}\langle Bu,u\rangle\right|\leqslant c'\|u\|^2. \tag{123}$$

Thus for $\lambda>c'+\hat{\lambda}$,

$$\|(L+\lambda I)u\|^2\geqslant\|Lu\|^2+\hat{\lambda}\|u\|^2. \tag{124}$$

Moreover, an elementary calculation using the system (77)–

(80) establishes that for λ_0 sufficiently large there exists d and $\bar{\lambda}$ so that, if $\lambda > \lambda_0$,

$$\|Lu\|^2 + \lambda \|u\|^2 \geq d\{\| - \nabla\tilde{p} + \nabla\times B \times B_0\|^2 + \|\nabla\times(\tilde{v}\times B_0\|^2 + \|\nabla\cdot\tilde{v}\|^2 + \bar{\lambda}\|u\|^2\}. \quad (125)$$

We define

$$L_{\bar{\lambda}} = L + \lambda I, \quad \bar{\lambda} > \lambda_0.$$

It is clear from the inequality (124) that the norm $\|L_{\bar{\lambda}}u\|$ is equivalent to the graph norm $\{\|L_{\bar{\lambda}}u\|^2 + \|u\|^2\}^{1/2}$ on D^+ and thus on the closure of D^+ in this norm. Thus to show that (113) is valid on all of $D(L_{\bar{\lambda}})$ we need merely to show that D^+ is dense in D. For now, assume we have proved this. We are then in a position to conclude the proof that $L_{\bar{\lambda}}$ is a closed operator.

Suppose that $(u_n, L_{\bar{\lambda}}u_n)$ is a Cauchy sequence in the graph norm. Since X is complete, there exist u, V such that $u_n \to u$, $V_n = L_\lambda u_n \to V$. We wish to show that $u \in D(L_{\bar{\lambda}})$ and $L_{\bar{\lambda}}u = V$. With $u = (\tilde{v}, \tilde{p}, B)$,

$$\nabla\times(\tilde{v}\times B_0), \nabla\cdot\tilde{v}, \nabla p - \nabla\times B \times B_0 \in L^2(\Omega), \quad (126)$$

$$\nabla\cdot B = 0 \quad (127)$$

are consequences of the continuity of differentiation in the sense of distributions. So we need merely to check that the boundary conditions $B\cdot n = 0$, $\tilde{v}\cdot n = 0$ are satisfied. As

$$\|L_\lambda u_n\| \geq c'\|B_n\|, \quad (128)$$

$B\cdot n = 0$ on $\delta\Omega$ is a consequence of the inequality

$$\|B\|_{H^{-1/2}(\Gamma)} \leq c\|B\|. \quad (129)$$

Similarly, from this inequality applied with u instead of B combined with the fact that

$$\|L_\lambda(u_n - u_m)\| \geq c'\|\nabla\cdot(v_n - \tilde{v}_n)\|, \quad (130)$$

we can conclude

$$\tilde{v}\cdot n = 0, \quad \text{on } \delta\Omega. \quad (131)$$

Thus $u \in D(L_{\bar{\lambda}})$, $L_{\bar{\lambda}}(u) = V$. Q.E.D.

We next would like to verify condition (2) and (3′) of the Hille–Yosida theorem. Condition (2), that the resolvent set $\rho(L_\lambda)$ contains (ω, ∞) for some sufficiently large ω, follows easily from a general argument that we outline here for completeness. First as $L_{\bar{\lambda}}$ is a closed operator, clearly the range of $L_{\bar{\lambda}}$ on $D(L_{\bar{\lambda}})$ is closed in X. Next we note that for λ_0's sufficiently large and real [possibly larger than λ_0 defined by (124)], (114) applies to the adjoint L_λ^* of L_λ to show that, if $\lambda' > \lambda_0'$, $u \in D(L_\lambda^*)$,

$$\|(L_\lambda' + \lambda' I)u\| \geq c\|u\|. \quad (132)$$

This shows that the range of $L_\lambda + \lambda' I$ is dense. For if it were not there would exist $V \in X$, $V \neq 0$, for which

$$\langle (L_{\bar{\lambda}} + \lambda' I)u, V\rangle = 0, \quad \forall u \in D(L_{\bar{\lambda}} + \lambda' I). \quad (133)$$

This would then be true in particular for $u \in C_0^\infty(\Omega)$. Taking into account the definition of $L_{\bar{\lambda}} + \lambda' I$ as a differential operator acting in the sense of distributions, this then implies $V \in D(L_\lambda^*)$ and

$$(L_\lambda^* + \lambda' I)V = 0, \quad (134)$$

which by virture of (132) implies $V = 0$. Last, we note that condition (3) of the Hille–Yosida theorem is satisfied by virture of inequality (113).

There remains only to prove the density. We recall the definition of $D(L_{\bar{\lambda}})$:

$$D(L_{\bar{\lambda}}) = \{u \in L^2(\Omega), - \nabla\tilde{p} + \nabla\times B \times B_0, \nabla\times(\tilde{v}\times B_0), \nabla\cdot\tilde{v} \in L^2(\Omega), \nabla\cdot B = 0, \tilde{v}\cdot n = B\cdot n = 0 \text{ on } \delta\Omega\}. \quad (135)$$

The technique in Ref. 18 applies (see Remark [4.2] and pp. 339–341). In outline one seeks to find approximating sequences that are defined on an open set $\Omega' \subset \Omega$. The elements of this approximating sequence can then in turn be approximated in Ω by first multiplying them by a function which is one on Ω and zero outside Ω', and then mollifying the result. To define the original sequence one uses the existence of an open covering of the set Ω and $\delta\Omega$ whose covering property is invariant under translations. For a more sophisticated approach under weaker hypothesis on the coefficients see Ref. 15. Then the translational continuity of $L^2(\Omega)$ does the rest.

We next would like to outline how to handle the cases (2) equilibrium with flow and (3) incompressible plasma.

Case B [equilibrium with flow (diffuse pinch)]: We first note that in the presence of flow, the equilibrium equations become

$$\rho_0 v_0\cdot\nabla v_0 = - \nabla p_0 + \nabla\times B_0 \times B_0, \quad (136)$$

$$v_0\cdot\nabla p_0 + \gamma p_0 \nabla\cdot v_0 = 0, \quad (137)$$

$$v_0\cdot\nabla S_0 = 0, \quad (138)$$

$$\nabla\cdot B_0 = 0, \quad (139)$$

and ρ_0 may be determined from (S_0, p_0) from the equation of state

$$p_0 = S_0\rho_0^\gamma. \quad (140)$$

The boundary conditions that are imposed are

$$B_0\cdot n = v_0\cdot n = 0, \quad \text{on } \Gamma. \quad (141)$$

We explain now how the special structure of the Lundquist equations makes possible the definition of a closed operator L on a domain that includes the boundary condition $\tilde{v}\cdot n = 0$, $B\cdot n = 0$.

First, we again define, for an appropriate λ,

$$D(L_\lambda) = \left\{ \begin{matrix} u \in L^2(\Omega), \quad L_\lambda u \in L^2(\Omega) \\ \tilde{v}\cdot n = 0 \quad \text{on } \delta\Omega, \ \nabla\cdot B = 0 \\ B\cdot n = 0 \quad \text{on } \delta\Omega \end{matrix} \right\}. \quad (142)$$

To see that this domain is closed in the graph norm we must show that the condition $\tilde{v}\cdot n = 0$ is satisfied. All the other steps are similar to those in the case of static equilibria.

Let

$$Lu = \begin{bmatrix} L_1 u \\ L_2 u \\ L_3 u \\ L_4 u \end{bmatrix}, \quad (143)$$

where L_1, L_2, L_3, L_4 correspond to $\tilde{v}_t$, B_t, $\tilde{p}_t$, and S_t, respectively. By definition,

$$L_2 u = \nabla\times\left(\frac{\tilde v}{\rho_0^{1/2}}\times B_0\right)+\nabla\times\left(\frac{\tilde v_0}{\rho^{1/2}}\times B\right). \tag{144}$$

Now given $\overline{B}$, note the identity

$$\begin{aligned}\nabla\cdot\left(\left(\frac{\tilde v}{\rho_0^{1/2}}\times B_0\right)\times\overline{B}\right)&+\nabla\cdot\left(\left(\frac{\tilde v_0}{\rho_0^{1/2}}\times B\right)\times\overline{B}\right)\\ &=\overline{B}\cdot\nabla\times\left(\frac{\tilde v}{\rho_0^{1/2}}\times B_0\right)-\left(\frac{\tilde v}{\rho_0^{1/2}}\times B_0\right)\cdot\nabla\times\overline{B}\\ &\quad+\overline{B}\cdot\nabla\times\left(\frac{\tilde v_0}{\rho_0^{1/2}}\times B\right)-\left(\frac{\tilde v_0}{\rho_0^{1/2}}\times B\right)\cdot\nabla\times\overline{B}.\end{aligned} \tag{145}$$

Integrating over Ω and using the divergence theorem we obtain for the left-hand side of (145)

$$\int_\Gamma\left[\left(\frac{\tilde v}{\rho_0^{1/2}}\times B_0\right)\times\overline{B}\right]\cdot n\,ds+\int_\Gamma\left[\left(\frac{\tilde v_0}{\rho_0^{1/2}}\times B\right)\times\overline{B}\right]\cdot n\,ds, \tag{146}$$

which, upon being expanded and using the conditions $B\cdot n = B_0\cdot n = \tilde v_0\cdot n = 0$, yields

$$\int_\Gamma(\tilde v\cdot n)B_0\cdot\overline{B}\,ds. \tag{147}$$

Choosing now $\overline{B}=\alpha B_0$, with $\alpha\in H^{1/2}(\Gamma)$, such that $\|\alpha\|_{H^{1/2}(\Gamma)}\geqslant c\|\alpha\|_{H^1(\Omega)}$, we find from (125) and (145) that

$$\left|\int_\Gamma(\tilde v\cdot n)B_0^2\alpha\,ds\right|$$

$$\leqslant c\{\|B_0\|_{L^\infty}\|\alpha\|\}\,\|L_2u\|+\|\nabla\times\overline{B}\|\,\|u\| \tag{148}$$

$$\leqslant c\{\|\alpha\|\,\|L_2u\|+\|\nabla\alpha\times B_0\|_2\|\tilde v\|+\|\alpha\|\,\|\tilde v\|\} \tag{149}$$

$$\leqslant c\{\|\alpha\|\,\|Lu\|+\|\alpha\|_{H^1(\Omega)}\|u\|\} \tag{150}$$

$$\leqslant c\{\|\alpha\|_{H^1(\Omega)}\|Lu\|+\|u\|\} \tag{151}$$

$$\leqslant c'\|\alpha\|_{H^{1/2}(\Gamma)}\{\|Lu\|+\|u\|\}. \tag{152}$$

Thus, by duality,

$$\|\tilde v\cdot nB_0^2\|_{H^{-1/2}(\Gamma)}\leqslant c'\{\|Lu\|+\|u\|\}. \tag{153}$$

Now since $B_0^2\tilde v\cdot n=0$ in $H^{-1/2}(\Gamma)$ implies $\tilde v\cdot n=0$ in $H^{-1/2}(\Gamma)$ (given that, by assumption, $B_0^2\neq 0$ on Γ), we see that condition $\tilde v\cdot n=0$ is preserved by this norm.

Case C (incompressible plasma): Here we add the condition $\nabla\cdot v=0$ in Ω. In this case it is not appropriate to make the change of variables (75) and (76). We use only

$$\tilde p=(\gamma p_0)^{1/2}p. \tag{154}$$

This transformation puts the system (77)–(80) into the form

$$(\rho_0 I)u_t+A_i'\frac{\partial}{\partial x_i}u+B'u=0, \tag{155}$$

with symmetric A_i', or

$$\begin{aligned}&u_t+A_i''\frac{\partial}{\partial x_i}u+B''u=0,\\ &A_i''=(\rho_0 I)^{-1}A_i,\quad B_i'=(\rho_0 I)^{-1}B_i'.\end{aligned} \tag{156}$$

Thus A_i'' are also symmetric. It is now easy to prove that

$$L_\lambda=-A_i''\frac{\partial}{\partial x_i}+B''+\lambda I \tag{157}$$

generates a semigroup. The boundary conditions $v\cdot n=B\cdot n=0$ on $\delta\Omega$ now both are preserved in the graph norm due to the inequality (50) and the fact that $\nabla\cdot v=\nabla\cdot B=0$.

V. COMPARISON OF THE DOMAINS

We here compare the domains of the operators corresponding to the second- and first-order formulations for the case of the diffuse pinch.

As our notion of a solution to the second-order equations, as discussed in Ref. 3, is to associate with them a second-order evolutionary variational problem following the work of Lions–Magenes,[12] the solution is thus defined in a space of functions requiring L^2 restrictions on only the first-order derivatives. This is what accounts for the similarity between the domains (48) for the second-order and (135) for the first-order (symmetric hyperbolic) formulations. As is clear from these definitions, the space defined for the first-order theory is such that its first component $\tilde v$ lies in the space W defined for the second-order theory. If, instead of v, we require, as discussed in the Introduction, that $\xi\in W$, and define p, B, which are denoted in (2) by $\bar v$, by

$$\begin{aligned}p&=-\xi\cdot\nabla p_0-\gamma p_0\nabla\cdot\xi+g_1(x),\\ B&=\nabla\times(\xi\times B_0)+g_2(x),\end{aligned} \tag{158}$$

we see that our notion of solution for the second-order equations yields p and $B\in L^2(\Omega)$. However, the conditions inherent in (135) when appropriately decoupled require more of p and B. For example, consider the condition

$$-\nabla p+\nabla\times B\times B_0=f\in L^2(\Omega). \tag{159}$$

Take the curl of both sides in $D'(\Omega)$ to get

$$\nabla\times(\nabla\times B\times B_0)=\nabla\times f\in H^{-1}(\Omega). \tag{160}$$

From the vector identity (valid in D')

$$\nabla\times(a\times b)=b\cdot\nabla a-a\cdot\nabla b-b\nabla\cdot a+a\nabla\cdot b, \tag{161}$$

we deduce

$$B\cdot\nabla(\nabla\times B)\in H^{-1}(\Omega). \tag{162}$$

Also, take the dot product of (159) with B_0 to obtain

$$B_0\cdot\nabla p=B_0\cdot f\in L^2(\Omega). \tag{163}$$

The uniqueness of solutions to (89) and (90) guarantees that there will exist $g_1(x)$ and $g_2(x)$ (which amounts to choosing an appropriate subset of initial data) for which (159) and (163) hold. A direct not functionally dependent definition of the appropriate g_1's and g_2's does not appear to be available, however. As is clear from the above discussion, however, $f=g=0$ will not ensure that (159) and (163) hold.

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ERRATA

Erratum: The most general magnetized Kerr–Newman metric [J. Math. Phys. 27, 562 (1986)]

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In Eq. (2.6), the sixth and seventh lines should read

$$-\beta\, arR \sin^2\theta\,[2(\alpha-\beta a)(\alpha-\beta a\sin^2\theta)+\beta(\alpha a-\beta(a^2+r^2))\cos^2\theta\,]\}$$
$$+4\delta(Eg-Be)R\cos\theta\{(\alpha-\beta a\sin^2\theta)[\beta^2(a^2+2\nu)\cos^2\theta-(\alpha-\beta a)^2]$$

Erratum: Structural analysis and elementary representations of SL(4,$\mathbb{R}$) and GL(4,$\mathbb{R}$) and their covering groups [J. Math. Phys. 27, 883 (1986)]

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On p. 885, right column, the two lines immediately preceding formula (2.21) should read as follows:

C. The Weyl group $W(\mathfrak{g},\mathfrak{a})$

We define for every $\lambda_k\in\Lambda^+$ a vector $H_k\in\mathfrak{a}$ by

